GDTk CHANGELOG 2024-q{:}

A newsletter for the GDTk Community

18 April 2025

My goal for a regular newsletter in 2024 was eclipsed by the frenzy of activity we had, which is a good thing! I'll attempt to capture the highlights of 2024 in a single newsletter, this one. So on that note, strap in!

Farewell to Volker Hannemann

Volker Hannemann from the German Aerospace Center (DLR) visited the compressible flow CFD group at UQ for a 6-month period from August 2023 to January 2024. In that time, Volker was an active participant in our morning tea discussion, dubbed CFTeaTime. As a research activity, Volker worked on a modification to the two-equation $k-\omega$ turbulence model that accounts for the presence of shocks (and so mitigates spurious production of turbulent kinetic energy). The modelling was integrated into Eilmer and contributes two parts: a shock detection method that is modelled as a transport process; and the modification of $k-\omega$ source terms in the presence of a detected shock.

The first farewell activity was an end-of-year breakup with Lightning Talks at the UQ city venue followed by a lunch of korean fried chicken. At the morning talks, we were also joined by a long-standing friend of the GDTk community: Monika Hannemann. For lunch, Volker's partner Annegret also joined us in the city.

On 18 January, Volker presented what he'd been up to during his visit at the Centre for Hypersonic Thursday talks. The slides from Volker's talk are hosted on the GDTk website along with the collection of presentations (and you can click the image in the margin to take you to the slide deck). Figure 1, a slide from Volker's talk, gives some indication of the turbulence modelling problem that Volker was addressing. A common problem with RANS turbulence models in a compressible flow is that there is an unphysical production of turbulence computed by the model. The Eilmer implementation of a standard $k-\omega$ model shows this in the top image. Volker implemented and adjusted a model by Rathi and Sinha¹ that attempts to mitigate the issue of unphysical turbulence production: the result of that work is in the bottom image in Figure 1.

On the Australia Day public holidy (26 Jan 2024), we all gathered at my place for a farewell BBQ for Volker and Annegret. The weather was decidedly odd and for most of the day we were wrapped in a blanket of cloud. Nevertheless, we enjoyed an afternoon of Australian-themed food and drink such as pavlova and lemon myrtle ice tea.





'Rathi & Sinha (2023) AIAA Journal 61(8) pp. 3337-3352



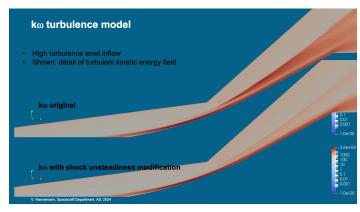


Figure 1. Slide 21 from Volker's talk shows a comparison of the turbulent kinetic energy field between the standard $k-\omega$ implementation and the modification that accounts for the presence of shocks.

Invited Lecture at the Von Karman Institute for Fluid Mechanics

In the late part of 2023, we received an invite to present Eilmer as a tutorial introduction at the Von Karman Institute of Fluid Mechanics as part of their lecture series on Advanced Computational Fluid Dynamics Methods for Hypersonic Flows. This was a great opportunity but it put a much harder deadline on the public airing of the Eilmer v5 release; I didn't want to present Eilmer4 (for which I had presentation materials) and then finish with the disclaimer that Eilmer v5 was on its way. This deadline made for a fun and intense GSoC (GDTk Summer of Code) to get everything prepared for the lecture series, taking place in the week before Easter. It even involved some Sunday Sessions for Peter and me: the coding type, not the pub type.

We made the deadline — even if it did involve me writing slides in the hotel room after feasting on mussels when I got to Brussels. You can find links to the lecture notes and the slides in this margin. The tutorial was well received, I feel, despite being the final talk on a Friday at the end of a long week.

It might come as no surprise but in a lecture series focused on hypersonic CFD, the dominant issue still in 2024 is to do with how the shock is resolved. Russell Cummings opened the lecture series with a history of CFD for hypersonic flow simulation, and made the point that most algorithms we still use were designed by the transonic flow simulation community. The subsequent lecturers each presented various tips or techniques for dealing with the simulations involving shocks. The suggestions included:

- careful grid construction and shock-aligned grids (Heath Johnson)
- better finite-volume numerics to capture dimensionality effects (Pierre-Henri Maire)
- using immersed boundary methods so that grid quality is less of an issue (Stefan Hickel)
- using shock-fitting and tracking to give a numerically clean representation of shock jumps (Aldo Bonfiglioli)





- using discontinous Galerkin methods as means for higher order simulations (Jaime Peraire)
- use of mesh adaption to get a non-uniform distrubtion of cell size where needed for resolution (Georg May)

Of course, what you choose today still remains a horses-for-courses type decision.

After the week-long lecture series, I took the opportunity to study Brussels' fine offerings of incompressible fluids. (Someone told me they have chocolate too — I wouldn't know.) Long-time GDTk member Jimmy-John Hoste acted as my guide. Thanks J-J! I received some experiential learning in the study of Belgian beers, and on the whole it was quite pleasant. As a bonus, I even made it on time to my return flight to Brisbane on the Saturday afternoon.



Figure 2. RJG enjoying the local culture in Brussels with GDTk member Jimmy-John Hoste.

GDTk team present at HiSST in Busan, Korea

The 3rd International Conference **High-Speed** Vehicle **Science** and **Technology** (HiSST 2024) was in held in Busan, Korea from 14 to 19 April 2024. Three members from the GDTk team went to participate and present at the conference: Nick, Rob and Amir.

Nick Gibbons presented his work on direct numerical simulation of supersonic mixing layers. Amir Mittelman spoke about his work on gradient-based multidisciplinary design, analysis and optimisation for high-speed vehicles. Rob Watt showed his work applying a four-temperature model to high-enthalpy conditions of the T4 shock tunnel nozzle.

The conference was a chance to catch up with old friends (see photo in Figure 3), and meet new ones. The team meet Jianshu Wu who had been using Eilmer as part of his Master's thesis in Korea.







Figure 3. GDTk community members at HiSST 2024. (You may spot a recurring figure. I swear this newsletter is not doubling as a Where's Wally publication.)

First Eilmer Workshop Day

On the 10th of July 2024, we hosted the first Eilmer Workshop Day at UQ's St Lucia Campus. The Eilmer dev team decided that it would be useful to present Eilmer v5 to SEQ local users and discuss the steady-state solver since it was getting a lot of use before its official release.

The workshop day had four parts:

- 1. RJG presented an overview of Eilmer v5 (based on the VKI tutorial) and a live demo on Eilmer v4 to v5 migration
- 2. User's showcase: members of the Eilmer community were given 5 minutes each to describe their research and how they were using Eilmer to help that. There were 14 presenters.
- Presentations on the Newton-Krylov solver. KAD gave the theoretical overview, and NNG presented examples and an experience report.
- 4. Ask-an-expert session. We finished the day with the dev team and advanced users helping others in the room with specific queries on using Eilmer.

The program for the day's events is on our github org page under gdtk-uq/eilmer-workshops.

Final PhD Seminars in CfH Seminar Series: Reece and Christine

In a luck of timing, we had two GDTk team members present their Final PhD seminars in UQ's Centre for Hypersonics seminar series in August 2024: Christine Mittler spoke to the group on the 1st of August, and Reece Otto on the 8th.

Christine presented her development of the Spatz flow solver. Spatz is a specialised flow solver that runs on CPUs and GPUs (that run CUDA-compiled code) to solve the compressible Navier-Stokes equations in 2- and 3-dimensions on non-uniform Cartesian grids. It has a shockcapturing operation mode that uses second-order reconstruction with limiting and makes use of conventional flux calculators in that mode. Spatz has a second operation mode that can be used for smooth flow regions. This is the higher-order mode that makes use of a 4th-order fluxreconstruction method. It is this mode that enables efficient direct numerical simulations to study high-speed boundary layers. Christine has applied Spatz to study how wall temperature affects the frequencies of receptivity in high-speed boundary layers. This knowledge helps understand how transition-to-turbulence will be affected by hot-wall structures for hypersonic vehicles (as opposed to traditional ground-based coldwall experiments). Some simulation results for the high-speed flow at Mach 7 over cold- and hot-wall flat plates in shown in Figure 4.



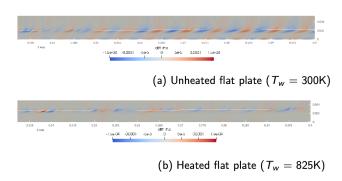


Figure 4. Spatz simulations using GPUs. These are unsteady calculations of high-speed boundary layer development in the presence of imposed noise for cold- and hot-wall conditions. See Christine's seminar slides for further details.

Reece presented his work on adjoint-based aerodynamic shape optimisation (ASO) in the presence of high-speed flows on August 8. Reece's thesis has focused on improving methods for adjoint-based optimisation. Two key improvements have been a rigorous treatment of 3D geometry modelling, and a design surface parameterisation technique that is well behaved for optimisation routines and propagates the surface changes into the volume grid in a mathematically-elegant and robust manner. Reece has called his adjoint-based ASO tool haste. These new capabilities for 3D aerodynamic shape optimisation have allowed Reece to study the optimised design of a hypersonic lifting body. As part of demonstrating the techniques (as opposed to attempting to model the physical reality), the method has been exercised for a range of fluid dynamic models for the aerodynamics: Newtonian-like panel methods, Euler equations, Navier-Stokes equations and the Reynolds-Averaged Navier-Stokes eqations. An optimisation result for a hypersonic lifting body using the Euler equations as flow model is shown in Figure 5. To give some hype to this result: this is CFD-in-the-loop optimisation of 3D shape using 118 design variables and it gives a converged shape result using 47 design iterations. The complete design cycle is 2 h 50 mins on a single workstation (16 cores of an Intel Xeon Siler 4216 CPU).

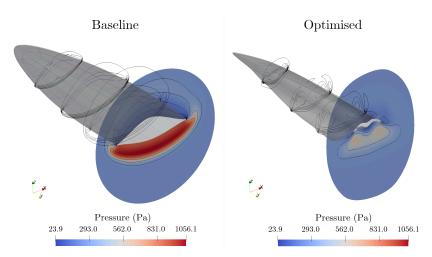


Figure 5. Haste + Eilmer aerodynamic shape optimisation result using an Euler model for flow. The optimisation goal was greatest lift-to-drag ratio that carried a segemented conical payload. Left: baseline configuration. Right: optimised configuration. See Reece's seminar slides for more details.

Winter Lightning talks

Christine and Rob organised the session for Winter Lightning talks. They took place on the afternoon of 16 August 2024. The order of speakers was randomly selected... except for Kyle. Kyle went last because he has rarely conformed to the 10-minute rule. Kyle's talk stood between us and the pub.

Nick G. I Can't Believe It's Not Adjoint: A Mystery Method for Com-

puting Flow Total Derivatives

Amir M. The GOAT

Shahzeb I. Film Photography: Analog Magic

Rowan G. Odin's Penguin

Seb v.O. The Art of Running

Christine M. Hopping between grids: The smooth moves of cubic spline in-

terpolation

Roshan K. Taking the Plasma Fuel Engine a bit too far...

Rob W. Acronym Spaghetti and Spaghetti Code: JFNK with (f)GM-

RES on GPUs

Carrie X. Different time-update methods for state-to-state modelling

Alex M. Typst: typesetting blazingly fast²

Kyle D. *Certainly, here is a possible title for your topic: "Algorithm*

Showdown: Unveiling the Power of Least-Squares - Normal

Equations vs QR Factorization"



Seb's talk involved how to game Strava art to produce an image of Bluey.

²The typst craze has since infiltrated the lab.

Farewell to Kyle Damm

Kyle finished his last day at UQ on 30 Sep 2024. He had been at UQ for 12 years, as a student then staff. Kyle had been a long-time principal developer for Eilmer, and worked on Eilmer in the transition to D-language years. In fact, Kyle's PhD thesis was the first one that was based on Eilmer v4: serving as the main development platform for his research into adjoint methods in a high-speed flow solver.

Kyle studied a BE in Mechanical & Aerospace Engineering at UQ from 2012-2015. He used and contributed to Eilmer v3 in his undergraduate thesis: developing and testing a GPU-accelerated chemistry module. He wrote that work up for presentation at the Australian Combustion Symposium in 2015, held in Victoria. There are some interesting historical notes associated with that project. We used OpenCL for the GPU implementation since it promised portability, and because CUDA felt too vendor specific at the time. Also, HPC-grade GPUs were a rarity in Queensland at the time. There were none available for undergraduate projects at UQ, for example. We made friends with the HPC team at QUT; they kindly gave us accounts on their high-performance computer so that we could access HPC-grade GPUs for testing.

Kyle studied for his PhD with the group from 2016-2019 (with conferral in February 2020). Kyle chose to work on CFD-based optimisation based on the adjoint method. Adjoint-based optimisation in CFD is an idea that goes back to Antony Jameson and has been reasonably well developed for low-speed flows. However, in high-speed flows with stronger shocks and more physics at play, adjoint solvers were few and far between. Access to a flow solver source code was critical for this study since adjoint-based optimisation is not a black-box optimisation method. Kyle submitted his thesis entitled Adjoint-based aerodynamic design optimisation in hypersonic flow in the September of 2019. A paper about the work was published in the AIAA Journal in 2020 and a result is shown in Figure 6. The work demonstrated the use of adjoint-based optimisation in a high-speed flow application, namely an inlet design, and that a somewhat complicated turbulence model could be used as an adjoint operator.

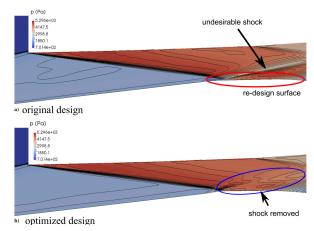
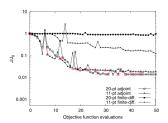


Figure 6. An adjoint-based CFD-in-the-loop optimisation of a hypersonic inlet using Eilmer.



Note the adjoint approach converges in far fewer iterations compared to a finite-difference approach (which one might do black-box style) and that the cost for the adjoint approach is effectively independent of the number of design parameters.

During Kyle's PhD, he embarked on some international collaboration in Korea. Kyle had a short research visit to Gisu Park's group at the Korean Advanced Institute for Science & Techonlogy, and a longer stay with Chongam Kim's group at Seoul National University. At the latter, Kyle was exposed to some other ideas and ways of doing to CFD development (which we attempted to disabuse him of on his return to UQ. (9)

As a postdoc at UQ, Kyle worked on several projects and most involved extending the capabilities of Eilmer. Kyle worked on new time-stepping routines for acceleration to steady-state and time-accurate marching such as local time-stepping and super time-stepping. Kyle also lead the development and simulation work for UQ's contribution to the BOLT II flight experiment. Kyle's coupled fluid-thermal simulations of the BOLT II configuration are still in use as eye candy on the website and in presentations.

Kyle's main contribution to Eilmer development was the Newton-Krylov solver based on complex-step differentiation and associate preconditioners. I suspect this will be an enduring contribution to the code base. A big motivator for building Eilmer v5 was to rework the code to accommodate the N-K solver once the algorithm had matured. We have pretty much completed that work (aside from the *small* job of documentation ³).

Kyle has now moved to the United Kingdom for his new job as Senior HPC Computational Engineer in the Advanced Computing Department at the UK Atomic Energy Authority. He tells me interacts with codes and teams that operate at slightly larger computational scales than the typical Eilmer calculation. Nevertheless, I'm sure the development skills he picked up with the GDTk group are serving him well.

We will miss Kyle and some of his spicy Lightning Talks. We hope he can visit the group when his travels bring him through Brisbane.

Tweets from the Aviary

Here are highlights from some of the flow codes associated with GDTk

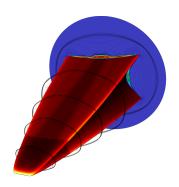
Steady-state Shock-fitting in Ibis

Rob did some proof-of-concept work in Ibis to test out an idea about how we could do shock-fitted boundaries in a Newton-Krylov solver. To do that, Rob added some new tech to Ibis: grid motion terms in the core equations; inverse-distance weighted grid deformation; a shock-fitting boundary condition; and a flexible GMRES preconditioner for the linear system solver to help with inclusion of flow properties and grid positions in the system of unknowns.

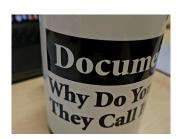
This worked out great and we've been able to modify the core ideas for inclusion in Eilmer. There will be more on that in the next newsletter since that's a 2025 feature for Eilmer.



Part of the BOLT II team (Kyle in centre, back) being interviewed by UQ News.



Coupled fluid-thermal simulation of the BOLT II flight experiment. Surface is painted with temperature map. Exit-plane contour is turbulent viscosity. Gray scale contour slices show pressure.



³Please see the advice on my favourite green tea mug.

Document it? Why do you think they call it code?

Largest calculation by GDTk group member and it's not on a supercomputer!

We have a new record in terms of largest cell count by a GDTk team member using GDTk codes: a quarter billion finite-volume cells. You can see there's a bit of qualification on that statement because I don't have complete awareness of how Eilmer is being used all over the world. In the 2023-q1 newsletter, we reported on Lachlan Whyborn's record-breaking calculation with Eilmer: 83.4M cells. That was on a high-performance cluster computer and used 1920 CPU-type cores.

Christine Mittler has raised the bar with a calculation done with her Spatz code. Spatz runs on both CPUs and GPUs. For this calculation, Christine loaded an 80GB NVIDIA H100 GPU with 248M cells and simulated a microsecond of flow in 4.2 hours of wall-clock time. Although Spatz is specialised in a manner that reduces its memory footprint (compared to Eilmer), it's still remarkable to see a quarter billion cells on a single GPU. This is looking like routine high-speed DNS is in reach for the Australian-based university researcher and not exclusively the playground for those with access to world top 20 supercomputing facilities.

GDTk community at AFMC in Canberra

We had a good showing of papers and GDTk community members at the Australasian Fluid Mechanics Conference in Canberra from 1–5 December, 2024. The list of papers here is likely not exhaustive; it's based on my memory.

- Mittler, Gollan, Jacobs (P), A comparison of CPU and GPU performance for high-order finite-volume methods for simulation hypersonic flows
- Watt, Jacobs (P), Gollan, Imran, Comparison of GPU programming models for computational fluid dynamics
- Gibbons, Wheatley, Effect of oxygen enrichment in high Mach number scramjet inlets
- Xie, Gollan, Gibbons, Jacobs (C), Jacobs (P), Investigation of non-Boltzmann distribution in hypersonic nozzle flows of nitrogen
- Ananthapadmanaban, Wallington, Hopkins, Gibbons, Toki, Scalo, Gildfind, James, Mee, Veeraragavan, Investigation of post-shock fluctuation levels in non-equilibrium hypersonic flow conditions
- Lakshman, Mee, Jacobs (C), Jacobs (P), Veeraragavan, Numerical investigations of three-dimensional shock-wave/boundary-layer interactions at Mach 6 hypersonic flow
- Hornung, Jacobs, Gollan, Collision of two plates in a gas

I'm sure there were other talks that made use of the GDTk software. Please let me know.

At the end of the week, we met up with former team member Lachlan Whyborn. Lachlan has been living in Canberra for the past year or so since he now works at ANU. On display below is my terrible group-selfie skills.



Figure 7. GDTk catch-up at AFMC. (If anyone has a better photo, please send it to me.)

Eilmer (online) Meet-ups

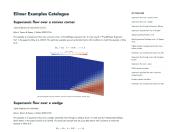
I already mentioned we had a busy year in 2024. This also affected the frequency of our Eilmer meet-ups. We met twice in 2024.

On 27 June 2024, we had what we a call a US-friendly meet up (based on the timezone differences). It was at 10am in Brisbane time. There was no guest speaker for that. Instead, I gave an update on what had been progressing with Eilmer v5 development.

Our second Eilmer User's Meeting was at the end of the year, once the team had arrived back from Canberra. This was a Euro-friendly meet up held on 12 Dec 2024 at 5pm (Brisbane time). At this meet up, Nick showed the new README file arrangement and how we're using that build a catalogue of examples to help navigate the new Eilmer v5 examples.

Summer Lightning talks to close the year

To finish the year, the group had their Summer Lightning talks on 20 December 2024 (which was the last working day of the year for most). For the second year running, we've headed to the city for the end-of-year lightning talks; it gives us a lot of options for a break-up lunch. The talk schedule is shown here:



The Eilmer v5 examples catalogue is assembled from the local READMEs in the source directories. In other words, every example in the catalogue has a matching directory in gdtk/examples/lmr. In August 2024, the dev team did a sprint month to add one new example per week each to the catalogue.

Summer Lightning Talks

Date: Friday, 20 December 2024

Venue: 308 Queen Street, Brisbane City; Rm 0G34 Heritage Creative Suite

Time: Arrival from 9:15am, start at 10:00am

Talk schedule

10:00a	Rob W.	One weird trick MPI doesn't want you to know about
10:15a	Amir M.	Send Science to Space, It's Awesome!
10:30a	Rowan G.	Computer-graphics-inspired CFD: Mean Value Coordinates
10:45a	Shahzeb I.	Grate Success: building a low-cost spectrometer
11:00a	Nick G.	The Worst Pokemon Speedrun Ever Attempted: An optimisation problem
11:15a	coffee/snack break	half hour refreshment break in Post Office Square (next to 308)
11:45a	Roshan K.	#A comment on shebang!
12:00p	Carrie X.	Speed Optimisation for Solving the 2D Convection-Diffusion Equation
12:15p	Alex M.	Duo(ble) Trouble
12:30p	Tristan V.	Magic Real Estate: How much land do I need?
12:45p	Seb v.O.	Can you hear the shape of a drum?
1:15p	lunch/drinks	end-of-year break-up

Late lunch

Venue: Pig 'n' Whistle Riverside (3 min walk from 308)

2025 Preview

At the time of writing this newsletter, it's April of 2025. Regardless, here's a preview of what's coming up in 2025. (And I hope to get the 2025-q1 newsletter out soon.)

- Eilmer v5 official release! We're close. We have: working code, a
 tutorial lecture, a reference manual, a catalogue of examples, builtin help in the command-line interface, and several presentations in
 our collection. We need to finish some user guides then we can
 ship.
- A new space-marching code in the collection: Pingvin.
- Eilmer in a benchmark exercise for the simulation of hypersonic flow over a flared cone geometry.
- International Shock Waves Symposium in Brisbane in July 2025. See GDTk community members Hans Hornung and Vince Wheatley deliver plenary lectures.

Eilmer v5 tip corner

I'd like to start a small section in the newsletter about Eilmer tips. So here goes.

The GDTk team is serious about reproducible research and has made an effort to make that easy for users of the code. When doing simulation work for research, you should be documenting your calculations by source code revision number and, even better, the details of the build environment. There are built-in lmr commands to help with that.



```
$ lmr revision-id
ef59f818
$ lmr revision-id --full
ef59f81839d82b80c32cc949106b4698cd68d003
$ lmr version
Eilmer 5.0 compressible-flow simulation code.
Revision-id: ef59f818
Revision-date: Sat Apr 5 08:14:15 2025 +1000
Compiler-name: ldc2
Build-date: Sat 5 Apr 2025 13:01:33 AEST
Build-flavour: debug
Profiling: omitted
Try going one step further and embedding the revision ID string in your
plots. Here's how I do that in GnuPLOT.
REV = system("lmr revision-id")
set label "[rev " . REV . "]" at screen 0.02,0.985
font ",10"
```

(and I'll ask for a user contribution for next newsletter to give a Python

COLOPHON

For this newsletter, I tried typst. It was produced using:

• typst, v 0.13.1

matplotlib example.)

• tufte-memo, v 0.1.2

