GDTk CHANGELOG 2023-q1

A newsletter for the GDTk Community

20 March 2023

Team visits Canberra for GPU Hackathon

contributions by Christine Mittler

In the last newsletter (`2022.q4`), we made mention of the GPU code `Chicken` and how that would be a platform for the team's participation in a GPU Hackathon in Canberra. Members from the compressible flow group at UQ were one of nine teams selected from across Australia to participate. Our team was: Nick Gibbons, Christine Mittler, Rob Watt and Peter Jacobs (see: photo of team with mentor Wei Fang)

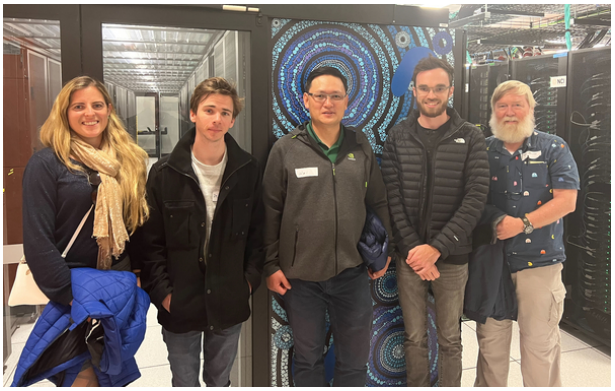

Figure 1: GPU Hackathon team in front of part of Gadi, supercompute cluster at NCI. *from left:* Christine Mittler, Nick Gibbons, Wei Fang (mentor), Rob Watt, and Peter Jacobs.

The hackathon was spread over five days. The first was Zoom-only with an introduction to the mentor Wei Fang. The second day was also online as preparation for the in-person event. The final three days took place in person in Canberra on 2,3 and 4 November 2022.

The team worked on development of `Chicken` with a particular emphasis to speed up simulation runtime by identifying and improving on performance bottlenecks. To do this, the team built up their skillset with NVIDIA code development tools. They worked with Wei Fang and other NVIDIA trainers to learn about profiling the code for performance and how to act on that information to enhance the code. Initial results from profiling revealed a few things: too much time spent copying data (at boundaries); and that the problem size was far too small to exploit GPU performance. After working on those low-hanging fruits, the team took a deeper dive into the performance of `Chicken` on GPUs. This deeper dive revealed that memory packing could be improved (in the jargon: there were uncoalesced memory accesses).

Over the three days of the hackathon, the `Chicken`'s simulation speed was improved by a factor of 5.

Record-breaking Eilmer calculation in 2022

contributions by Lachlan Whyborn

In 2022, a new record for largest Eilmer simulation was set; largest in terms of number of cells and compute hours. As part of Lachlan Whyborn's PhD, he simulated high-speed flow over a 3D slice (of 6 degrees) of a blunted cone. The structured grid had 7725 cells in the streamwise direction, 180 cells in the wall normal direction, and 60 cells spanwise. This was a total of 83.4M cells. The time-accurate calculation was split across 1920 cores and ran for 40 hours to simulate approximately 1.5 ms of physical time.

Lachlan used these simulations to study the difference between three-dimensional and two-dimensional effects on instabilities in hypersonic entropy layers. Prior to this calculation, the work was focused on axisymmetric simulations. The 3D simulations did reveal a difference in the physics: the hypersonic entropy layer is unstable to three-dimensional instabilities. The visualisation shown here is of density fluctuations. You can see mild disturbances in the shock layer, but focussing and amplification of disturbances in the entropy layer. The entropy layer edge is shown as the green line, and the boundary layer edge is the black line.

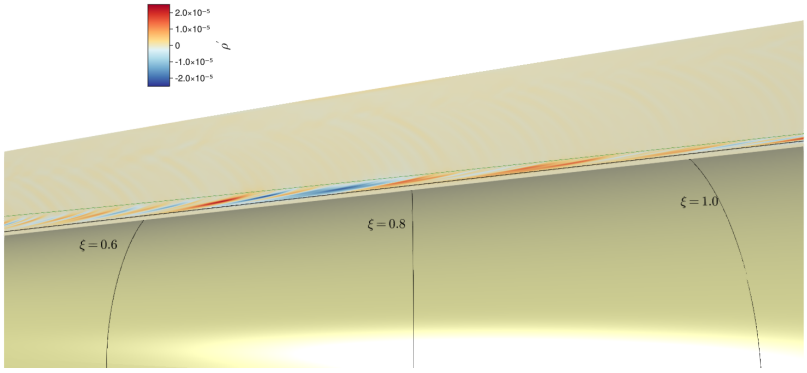

Figure 2: Instantaneous density fluctuations in the shock layer of high-speed flow over a blunted cone. The cone has a 7-degree half-angle, length of 1.2 m and a nose radius of 17.78 mm (0.7 in.). The free stream flow is at Mach 8. *Image supplied by Lachlan Whyborn.*

Visits to South-East Queensland

From September to December 2022, we hosted Friedrich (Fritz) Ulrich, our second PhD visitor from the Technical University of Munich. During Fritz' visit, he participated in our Lightning talks (more in next article); gave a talk in the CfH seminar series (10 Nov 2022); went on a visit to the hypersonics group at UniSQ; and attended the Australasian Fluid Mechanics Conference.

So that our visitors had some wider exposure to hypersonic activities in South-East Queensland, we organised a visit to the group at the University of Southern Queensland. The Brisbane-based people drove up the hill to visit UniSQ on Monday 28 Nov 2022. The timing was good — being a week out from the Australasian Fluid Mechanics Conference — for the groups to have a practice of their presentations. The photo below shows part of the group, and it's important to notice the back drop — that's right, the UQ people managed to find where the food is. (It's a long drive from Brisbane!)

Figure 3: Inspecting the hardware in the hypersonics lab at UniSQ.

Figure 4: Group visit to UniSQ. *from left:* Tamara Sopek (UniSQ), Byrenn Birch (UniSQ), Hiroki Sakamoto (Tohoku University), Friedrich Ulrich (Technical University of Munich), Yu (Daisy) Liu (UQ), and Peter Jacobs (UQ). *Image supplied by Christine Mittler (not in photo).*

Spring lightning talks

The group partook in another session of lightning talks in the tail end of Spring, on 18 Nov 2022. Lighting talks are strictly 10 minutes in length, although our timing may have been derailed by letting Kyle speak first. The topics are open for the presenter to choose. As a personal comment, I enjoyed the afternoon of talks and I learnt some new things. We were also fortunate that we only had two talks on AI! The list of presenters and topics is shown here.

Kyle Damm	Super(duper)-time-stepping
Lachlan Whyborn	The Cosmic Distance Ladder: the precarious ladder to deep space
Reece Otto	CAD to CFD: generating surfaces with holes or singularities
Jamie Border	Can I make fancy regression beat Eilmer?
Fritz Ulrich	I know that I know Nothing — working with AI
Peter Jacobs	BBQ Chicken: A Combustion Model for `Chicken`
Christine Mittler	Chicken-run in Canberra: a brief travel review
Amir Mittelman	Project Apollo: did they get it right?
Rowan Gollan	Books that helped me understand the "world"
Rob Watt	Banging my head against OpenMP
Daisy Liu	Numerical modelling of ionizing Saturn-entry shock layer
Nick Gibbons	`Perf`: One Profiler to Rule Them All

Figure 5: Lightning captured over Brisbane's Story Bridge. While the discussion was robust at our Lightning Talk session, I'm pleased to report it didn't get this heated.

Conferences recap

In December 2022, a few of us got to attend and present work at the Australasian Fluid Mechanics Conference (AFMC) held at the University of Sydney. Rob Watt's work on a three-temperature model for studying electron transpiration cooling was presented, and Lachlan Whyborn spoke about his work on fluid physics investigation of instabilities in high-speed boundary layers.

There was a good showing of hypersonics at the AFMC. Joanna Austin gave keynote talk about nonequilibrium effects in hypersonic double-cone flows. Richard Morgan was elected as Fellow to

the Australasian Fluid Mechanics Society. Members of the team got to meet avid Eilmer user, Hans Hornung, in person. Rob probably regretted that encounter moments later when Hans requested an implementation of a four-temperature model into Eilmer.

The AIAA SciTech conference was held at National Harbor, Maryland in the final week of January 2023. Four of us from the team travelled from East coast of Australia to East coast of the US to present: Jamie Border, Kyle Damm, Lachlan Whyborn and myself. Jamie presented his work on the use of Walsh functions for shock representation in finite-volume reacting gas dynamic simulations. Kyle presented at one of the special sessions for the BoLT-II flight experiment. Kyle talked on coupled fluid-solid heating simulations of the flight experiment, and the use of super-timestepping to accelerate time-accurate calculations of the heat soak into the solid domain (figure shown below). Lachlan showed his work on simulating 3D instabilities in the high-speed flow over a blunted cone. I gave a talk about our developments of a Jacobian-free Newton Krylov solver to accelerate steady-state convergence in hypersonic flow simulations.

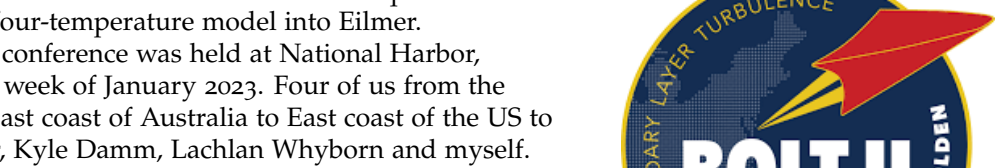

Figure 6: Kyle Damm's talk at SciTech was in the second of three special sessions related to the BOLT-II flight experiment.

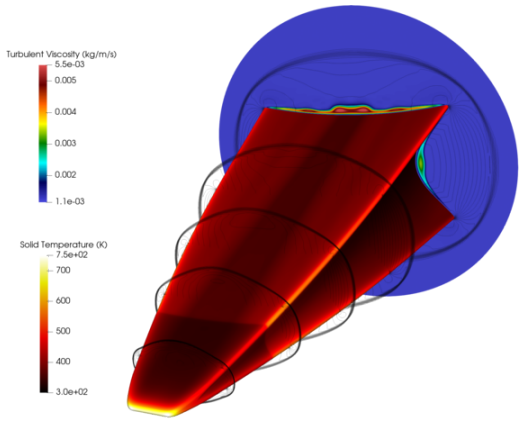

Figure 7: Coupled fluid-solid simulation of heating into BoLT-II flight article during descent portion of the trajectory. Solid surface is coloured with temperature field. Flow field contours are of turbulent viscosity. *Image supplied by Kyle Damm.*

Talking about Eilmer abroad

While travelling in the States, I took the opportunity to mix a bit of business and pleasure. By that I mean, I visited some universities that crossed my travel path.

In Tucson Arizona, I went to visit the hypersonics research group at the University of Arizona. I spent the afternoon of 24 Feb 2023 visiting their testing facilities and meeting with faculty. At the conclusion, I gave a seminar to the group about Eilmer and things we do with it. Specifically, I spoke on our Jacobian-free Newton Krylov development work and how we've used an adjoint solver for hypersonic aerodynamic shape optimisation.

In the following week, I visited Joanna Austin's research group at Caltech. I was hosted by Joanna and Hans Hornung for a 2-day visit on 28 Feb and 01 Mar 2023. On the first day, we had a session of informal talks where I got to learn what the PhD students are up to. After lunch, Dale Pullin gave me a tour of the Caltech campus. In the late afternoon of the first day, I presented a talk on Eilmer. It covered a general overview, the JFNK work[1] and application of Eilmer in the study of electron transpiration cooling for hypersonic

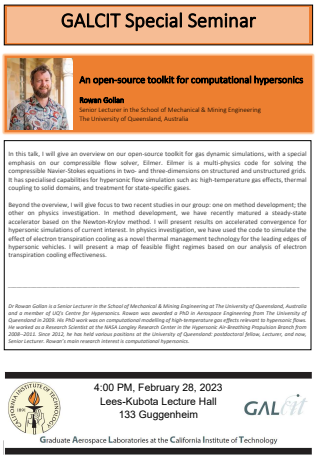

Figure 8: Advertising of my talk at Caltech.

[1] You may have noticed by now that I got my mileage out of preparing the JFNK talk for SciTech.

vehicles. On the second day, I met with students and faculty to discuss aspects of research. There was some odd weather while I was in Los Angeles, and you can make out the snow on the mountains in this view from the visitor's office (photo right).

Figure 9: Room with a view. The view from my visitor's office in Firestone building looking North.

Lorikeet

At the start of 2022, Peter Jacobs built a 2D space-marching code called Puffin. (You can find slides from a talk on Puffin at `https://gdtk.uqcloud.net/pdfs/gdtk-talk-pj-2022-mar.pdf`.) This exercise had at least two motivations: (1) an experiment in re-purposing the core gas dynamics routines into a simple-to-understand simulation program as an educational tool; and (2) as a rapid calculator for compression fields as a replacement to a much older NASA code (and no longer maintained), Seagull.

Enter Lorikeet: a 2D time-marching simulator for compressible flows. Peter built Lorikeet from the same core code as Puffin. In fact, to build and try Lorikeet, navigate to the Puffin source area. When you build Puffin, you get Lorikeet for free. Lorikeet differs from Puffin in terms of the types of flow. Lorikeet is time-marching and shock-capturing so it can handle unsteady flows and flows with big subsonic regions. On the other hand, Puffin is restricted to steady-flows that are predominantly supersonic (so that the space-marching assumption isn't pushed too far).

Building Lorikeet proceeds like this:

```
> cd gdtk/src/puffin
> make install
```

Figure 10: The new code is named after the Rainbow Lorikeet. This parrot is native to the Eastern seaboard of Australia.

Here we show a periodic shear layer simulated with Lorikeet. The contours show vorticity.

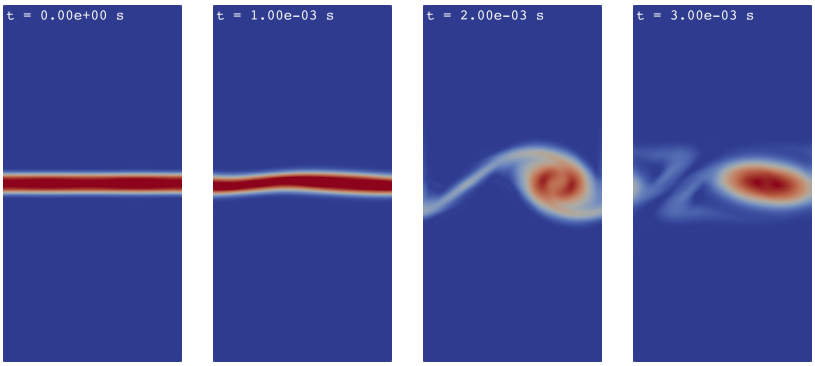

Figure 11: Vorticity contours in time sequence for a perioodic shear layer computed with Lorikeet.

Welcome!

In January 2023, two new PhD students joined the group. We'd like to welcome Caiyu (Carrie) Xie and Alex Muirhead. Both will be working with Eilmer and adding to its capabilities throughout their PhD studies. Carrie is looking at how to model highly nonequilibrium flows in the expanding portions of blunt bodies using state-specific models for population distributions. Alex will work on computing radiation fields for high-speed atmospheric-entry shock layers.