

Final presentation - 7 Dec (Thu)

# GPU Accelerated ~~Pressure Solver~~ ~~for~~ TIGER-F code



## Team Members

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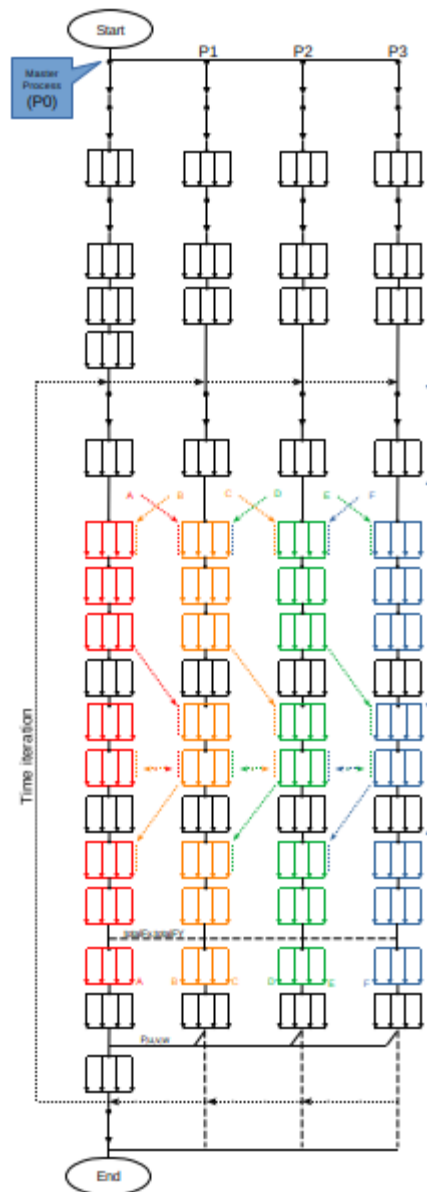
# TIGER-F

- Problem trying to be solved  
3D-CFD using the Direct Forcing Immersed Boundary (DFIB) method, LES turbulence model.
- Scientific driver for the chosen algorithm  
The flexibility to solve large scale FSI problems.
- What's the algorithmic motif?  
The use of simple and fixed Cartesian grids eliminates the need for remeshing, even as the structure is in motion.
- What parts are you focusing on?  
Initially: Computation intensive parts (pressure solver).  
But in the end, we need to offload all processes in the main iteration.

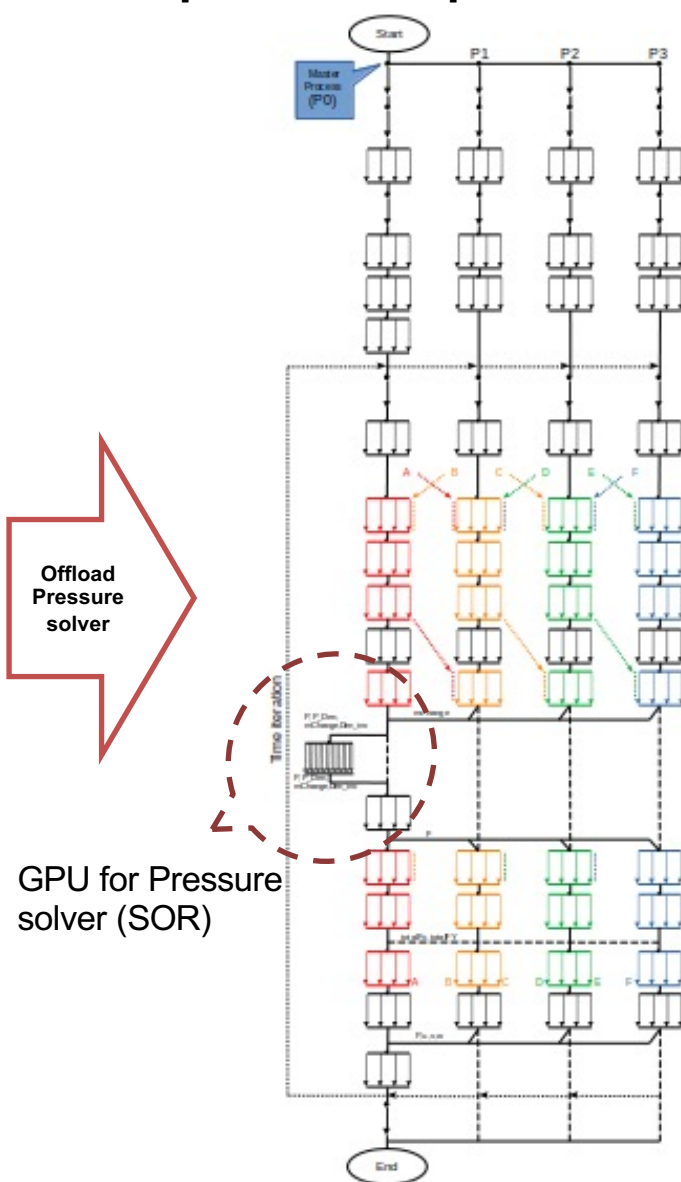
# Evolution and Strategy

- What was your goal coming here?  
to **speedup** our in-house solver using openACC by offloading and optimizing the computation intensive processes (e.g. pressure solver) into GPU
- What was your initial strategy?
  - To optimize the GPU-accelerated pressure solver and to use the Nsight systems for profiling.
  - to offload more subroutines into GPU.
- How did this strategy change?  
The majority of computational time is consumed by data transfer overhead, which could be diminished by relocating **all** processes into GPU.

## open MPI + openMP



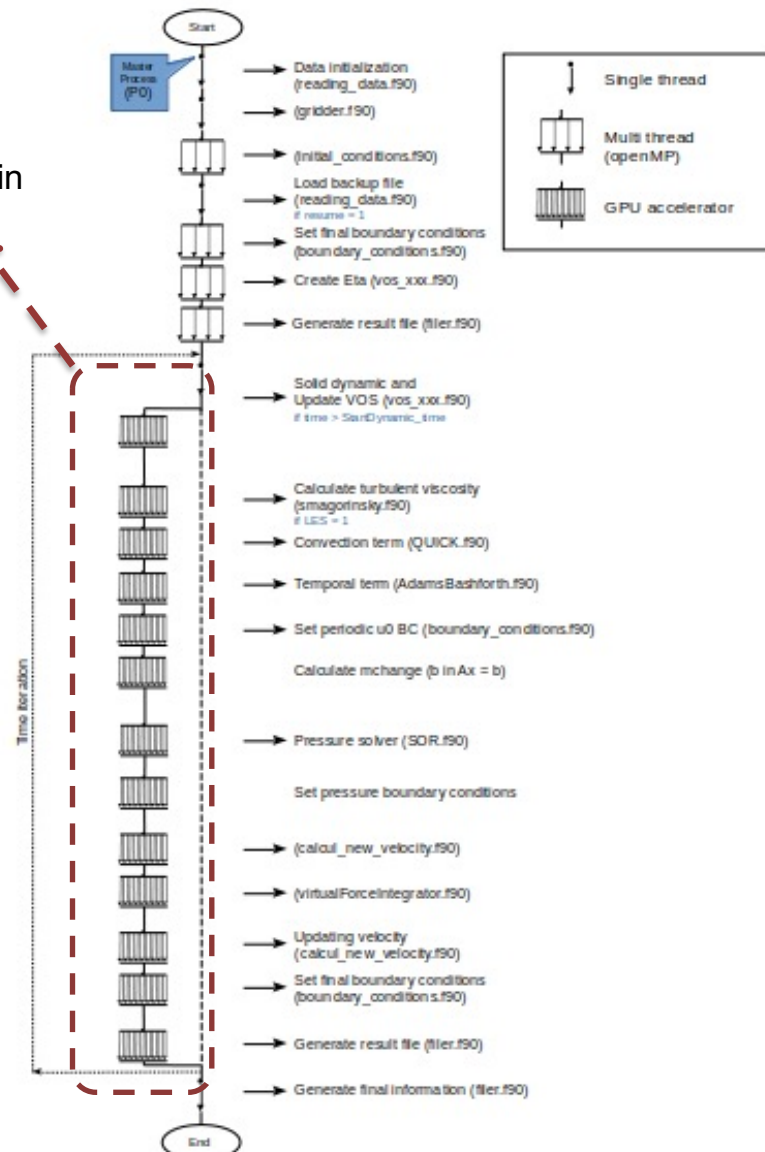
## open MPI + openMP + openACC



## openMP + openACC

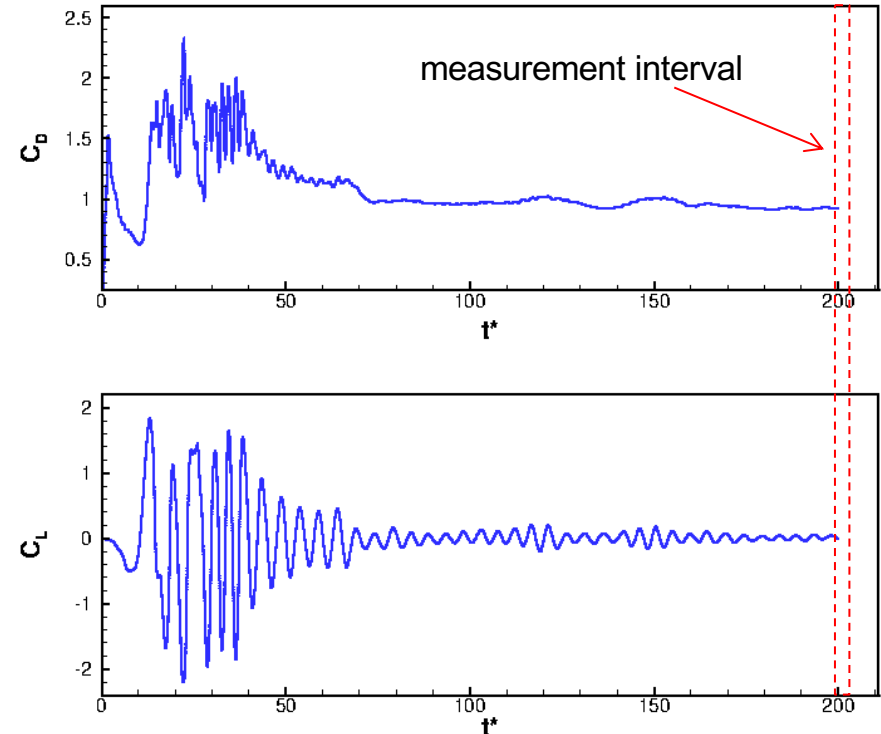
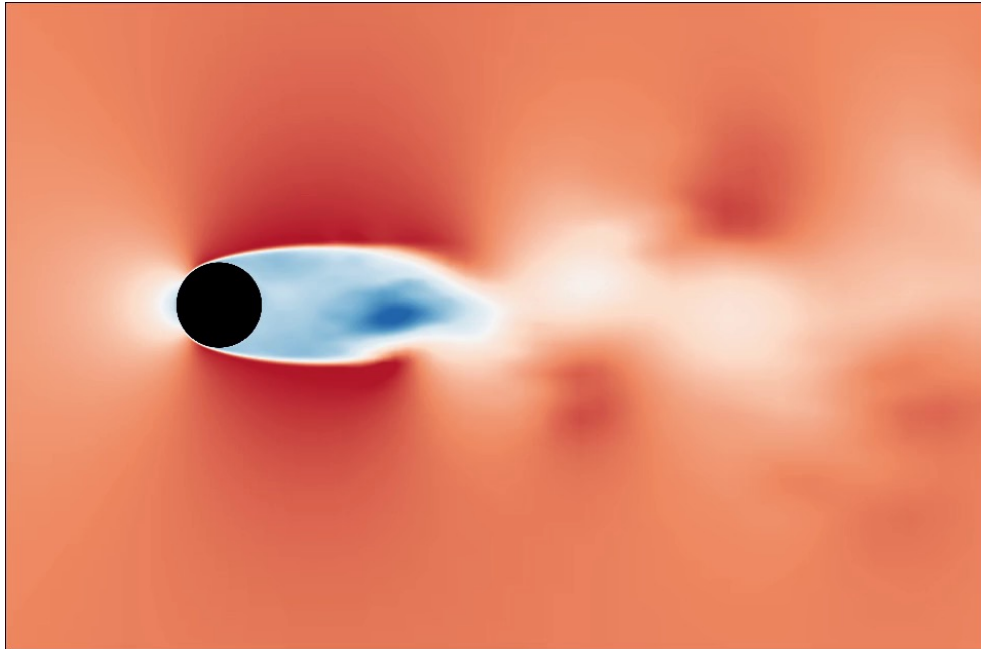
GPU for main iteration

Offload more into GPU

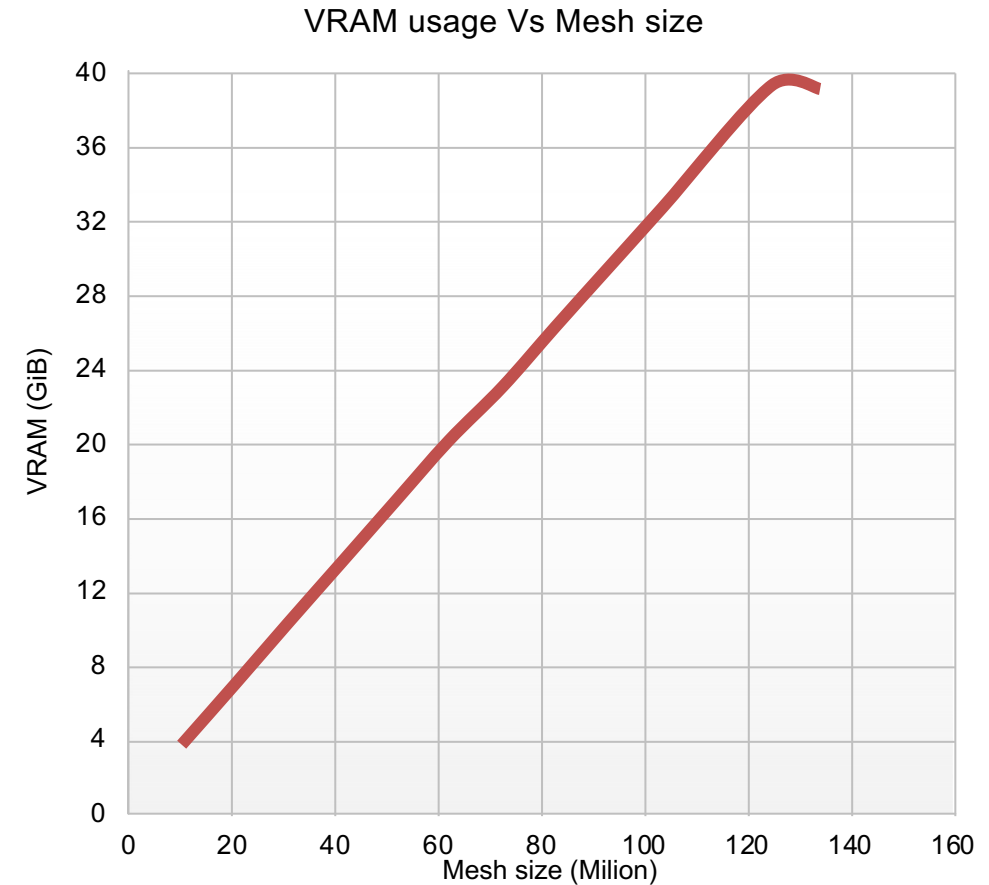
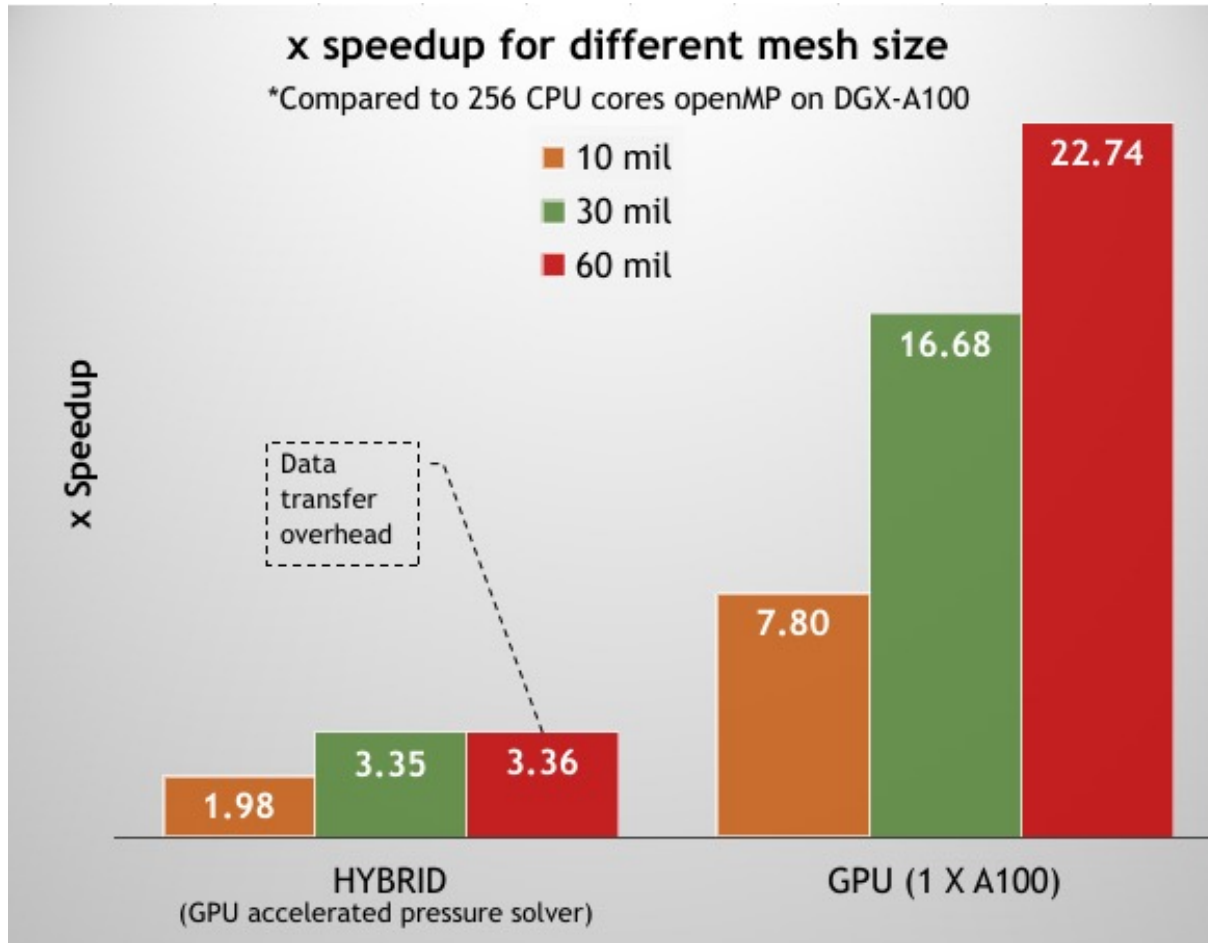


# Test Case

The test case was the flow past a stationary cylinder at  $Re = 5000$ , running for 200 sec of dimensionless time to give enough time to reach a **steady number** of pressure iterations. Speedup was measured for the next 1 second.



# Results and Final Profile



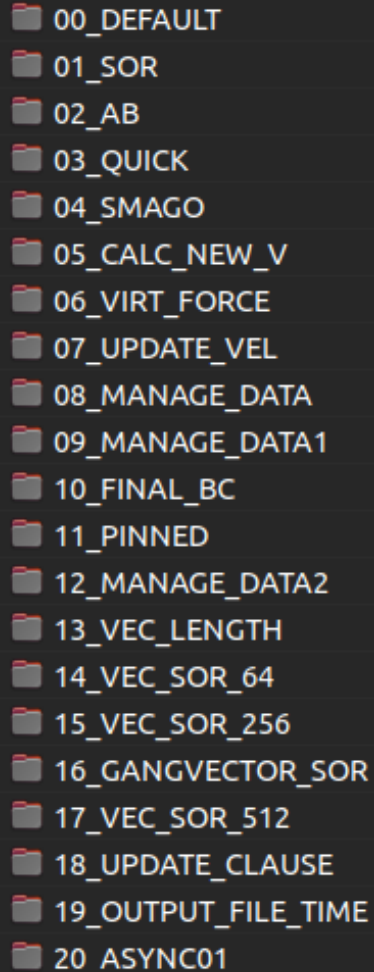
# Results and Final Profile

## What did you learn?

- Data transfer management.
- OpenACC's three levels of parallelism (gang, worker, vector).
- Profiling tools: Nsight systems, NVTX.

## Achieved new scientific goals?

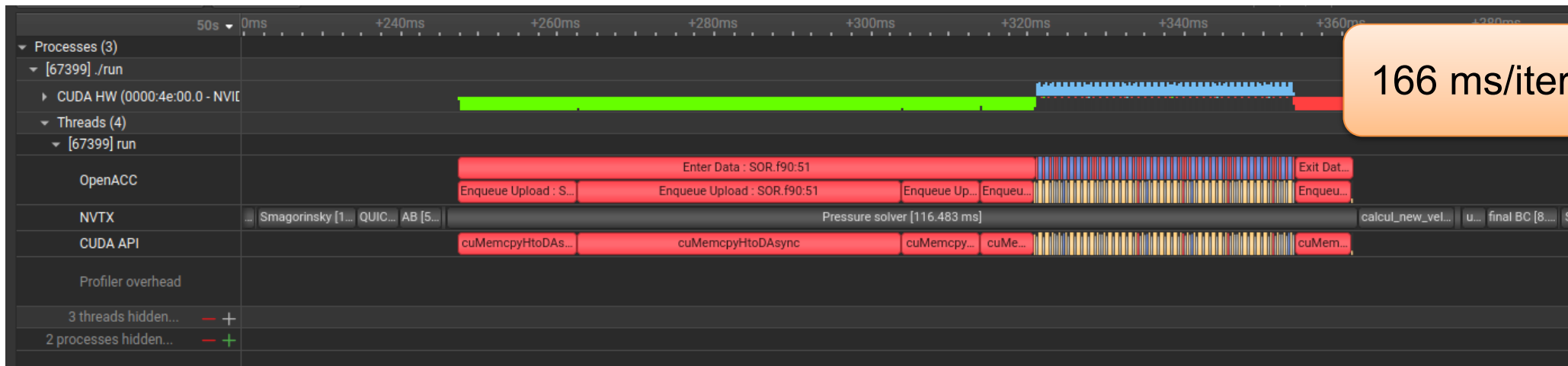
- Apply the red-black SOR algorithm for 3D domain, and run in GPU.
- 100 Million of mesh is possible to be done (very) much faster --> one step closer to simulate real world cases.



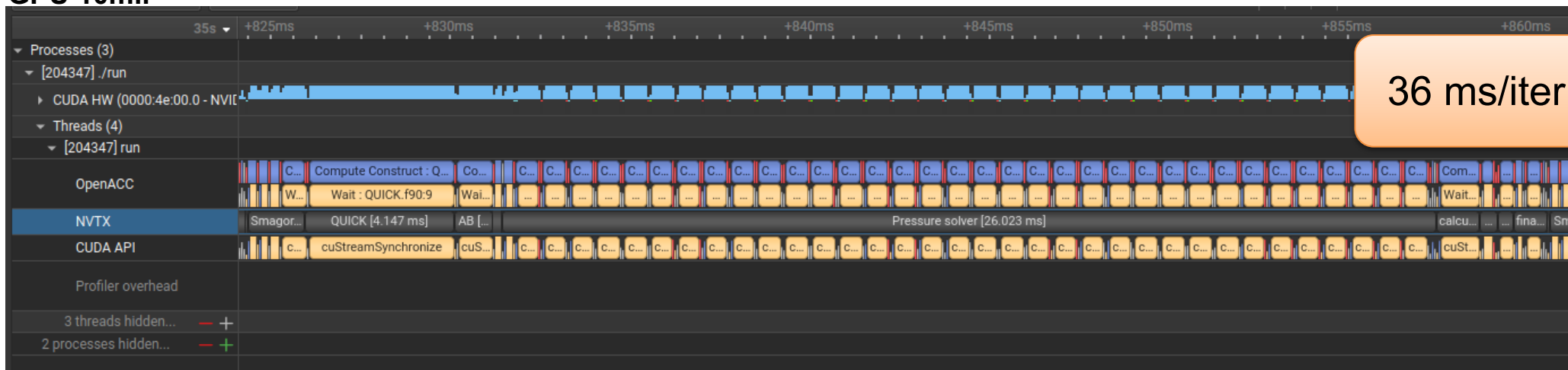
```
00_DEFAULT
01_SOR
02_AB
03_QUICK
04_SMAGO
05_CALC_NEW_V
06_VIRT_FORCE
07_UPDATE_VEL
08_MANAGE_DATA
09_MANAGE_DATA1
10_FINAL_BC
11_PINNED
12_MANAGE_DATA2
13_VEC_LENGTH
14_VEC_SOR_64
15_VEC_SOR_256
16_GANGVECTOR_SOR
17_VEC_SOR_512
18_UPDATE_CLAUSE
19_OUTPUT_FILE_TIME
20_ASYNC01
```

# Results and Final Profile

## HYBRID 10mil



## GPU 10mil





# Energy Efficiency

INPUTS	
# CPU Cores	256
# GPUs (A100)	1
Application Speedup	16.7x

Node Replacement	266.9x
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GPU NODE POWER SAVINGS			
	AMD Dual Rome 7742	8x A100 80GB SXM4	Power Savings
Compute Power (W)	293,568	6,500	287,068
Networking Power (W)	12,393	93	12,300
<b>Total Power (W)</b>	<b>305,961</b>	<b>6,593</b>	<b>299,368</b>

Node Power efficiency	46.4x
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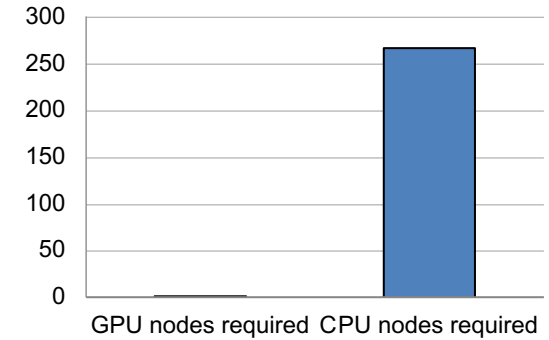
ANNUAL ENERGY SAVINGS PER GPU NODE			
	AMD Dual Rome 7742	8x A100 80GB SXM4	Power Savings
Compute Power (kWh/year)	2,571,656	56,940	2,514,716
Networking Power (kWh/year)	108,563	814	107,749
<b>Total Power (kWh/year)</b>	<b>2,680,219</b>	<b>57,754</b>	<b>2,622,465</b>

\$/kWh	\$ 0.34
Annual Cost Savings	\$ 891,638.13
3-year Cost Savings	\$ 2,674,914.39

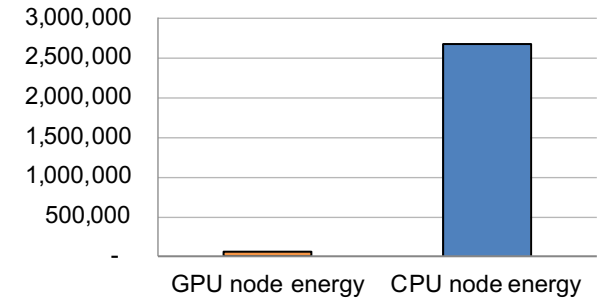
Metric Tons of CO <sub>2</sub>	1,859
Gasoline Cars Driven for 1 year	401
Seedlings Trees grown for 10 years	30,735

(source: [Link](#))

Nodes required for equivalent throughput

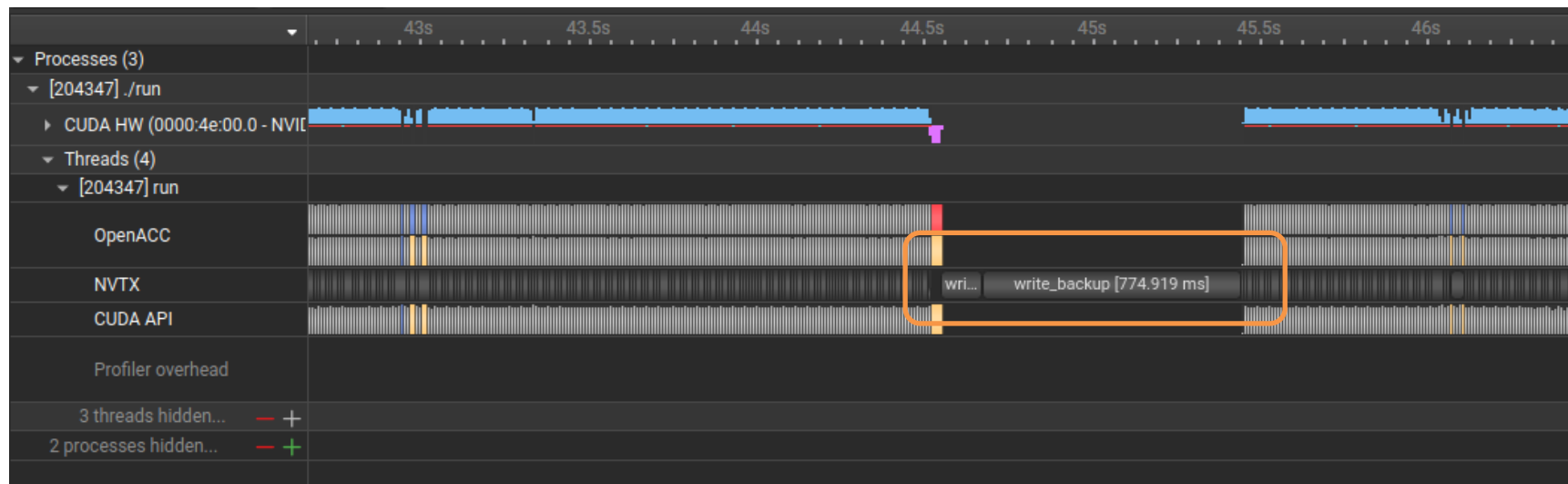


Annual energy required for equivalent throughput (kWh)



# What problems have you encountered?

- Unsuccessful Async between CPU file writing and GPU processes
- Unable to use “cache” clause
- Nsight compute could not be used because CAP\_SYS\_ADMIN capability was disabled.



# Wishlist

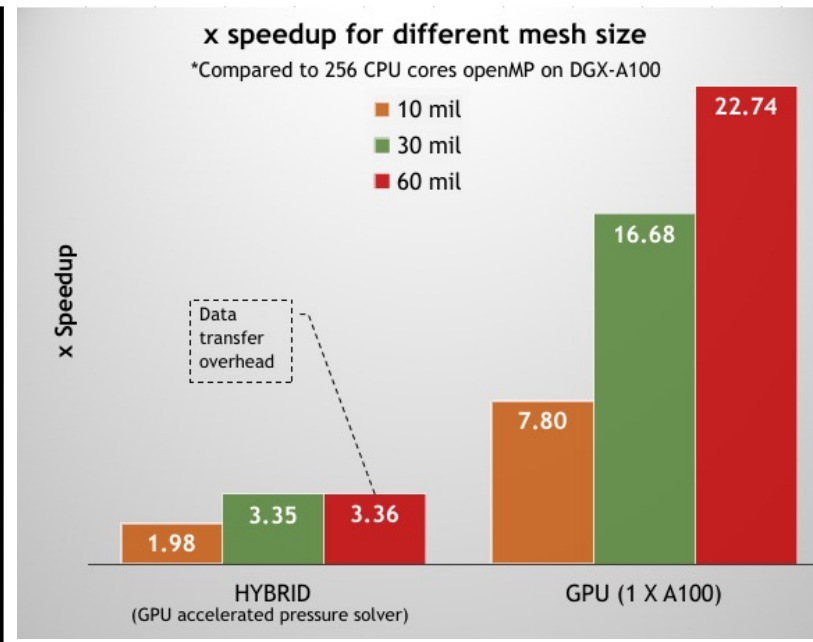
- What do you wish existed to make your life easier?
  - Multi GPU resource availability.
  - Updated training especially on multi GPU utilization.
  - An integrated cluster with a balanced CPU+GPU performance.

# Was it worth it?

- Was this worth it? Definitely YES!
- Will you continue development? YES
  - problems encountered on this event (async file writing, cache)
  - Use Nsight compute to optimize kernels
  - Multi-GPU process
  - Employing a readily available linear system solver with multi-GPU support. (AmgX)
- What sustained resources/support will be critical for your work after the event?
  - Multi-GPU resource and support.

## Application Background

- A 3D-CFD in-house code using the DFIB method, LES turbulence model.
- Pressure solver is the most computational intensive subroutine.



## Hackathon Objectives and Approach

- Offloading into GPU
- Reducing data transfer overhead
- Profiling / hot spots
- Performance tuning

## Technical Accomplishments and Impact

- Learn more openACC directives & clauses
- Learn how to use Nsight systems
- Offload more processes into GPU
- Reduce data transfer overhead
- Speedup

## Please use 100 words to summarize your team's achievements during this Hackathon

We began considering GPU offloading around 7 months ago and successfully accelerated our pressure solver onto the GPU. This hackathon not only boosted our learning curve but also enhanced the performance of our code. From this event, we are able to:

- Utilize openACC directives and their clauses
- Manage host-device data transfer better
- Optimize parallelism using openACC's three levels of parallelism (gang, worker, vector)
- Utilize Nsight systems with NVTX to profile the code
- Offload all processes in the main iteration to the GPU.
- **Achieve a speedup of 16.7x** (and even higher with increased computational load)

This marks another milestone for our in-house code as large-scale computations are required to simulate real-world cases. The significant speedup achieved is a substantial leap forward for us in reaching that goal.

# Thank You!

## Our mentors:

Bharat, Shijie, Kuan-Ting

Host	Jay	Floating Mentor	Bharat, Aswin
Host	CK	Marketing	Jinny
Infra Setup	Kuan-Ting	Event logistics	Apoorva
Account Manager	Vincent	NCHC Contact Window	Zhoujin Wu

All mentors and all participants in this hackathon

**NAR Labs** 國家實驗研究院

國家高速網路與計算中心

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