Scrum #1

NCHC X OpenACC X NVIDIA

OpenACC
More Science, Less Programming

2024 NCHC Open Hackathon

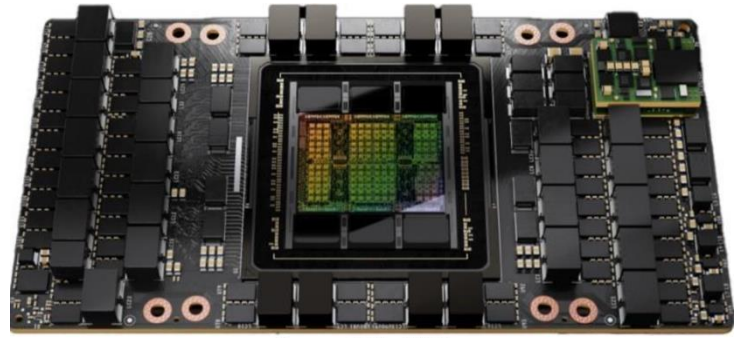
Important Dates

- 2024 / 10 / 15 (Tue) ： Registration deadline
- 2024 / 11 / 04~08 ： Connecting Mentors and Teams
  - Slack Channel, Emails Group, Line Group
- 2024 / 11 / 13 (Wed) ： Day 0: Kick-off Meeting 14:00~17:00 PM (Online)
- **2024 / 11 / 20 (Wed) ： Day 1: Scrum #1 Meeting 14:00~15:00 PM (Online)**
  - 4-minute presentation per team
- 2024 / 11 / 27 (Wed) ： Day 2: Scrum #2 Meeting 14:00~15:00 PM (Online)
  - 4-minute presentation per team
- 2024 / 12 / 04 (Wed) ： Final Day 10:00~16:00 PM (In-person at NCHC)
  - 12-minute presentation + 3-minute Q&A per team

H100 Resources

Slurm + Dockerless/Apptainer(Singularity)

- Prerequisite
  - Familier with Slurm + Dockerless/Apptainer(Singularity)
  - H100 matters to your project, for examples:
    - Accelerate with FP8 or DPX instructions
    - Benchmark A100 vs H100



Hopper GPU – H100

- Contact Jay Chen (Host) if got a plan to test on H100.

H100 Spec:
https://resources.nvidia.com/en-us-tensor-core/nvidia-tensor-core-gpu-datasheet?ncid=so-link-753678

Day 1 - Scrum #1 Meeting 14:00~15:00 PM (Online)

4 mins for each team

- #team-12-cycu-quantum
- #team-11-plantmen
- #team-10-smile-lab
- #team-9-gba-vvm
- #team-8-elsa-robotics
- #team-7-nolab
- #team-6-nthu_lsalab
- #team-5-parallel-minds
- #team-4-ntut_birdsong
- #team-3-氣象署-興大應數聯隊
- #team-2-nycu-hpc-team2
- #team-1-dream-chaser

淺顯易懂的標題

研究領域示意圖

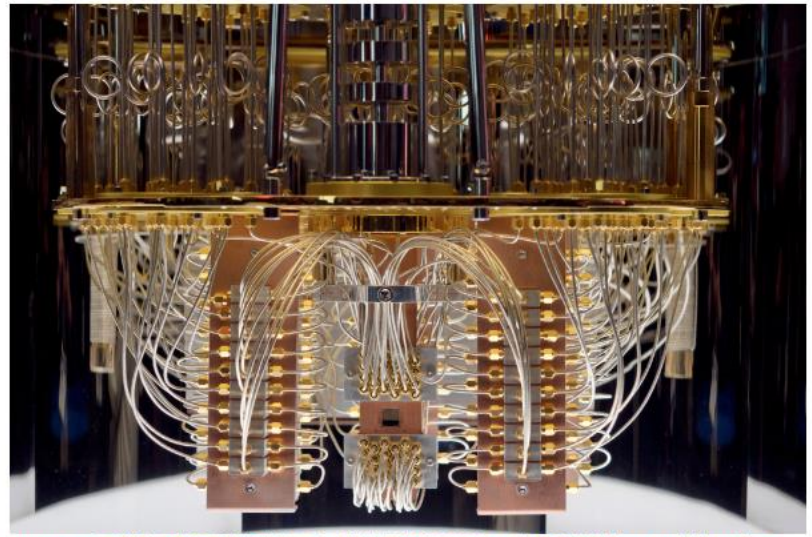
{__} 團隊來自 {__}老師帶領的{__}實驗室，將 {__} 加速了 {__} 倍！！

250~500 字儘量易懂的描述。
為什麼這個領域重要？為什麼這個命題重要？
加速成果？加速帶來什麼影響和潛力？

和加速成果相關的補充數據

報告投影片連結 (由國網上傳到 github)

量子算法模擬



haofan2023團隊成員來自臺灣大學資工系「洪士灝老師實驗室」，將量子演算法QAOA加速468倍！
— NVIDIA Mentors: Tian Zheng, Frank Lin, Yun-Yuan Wang

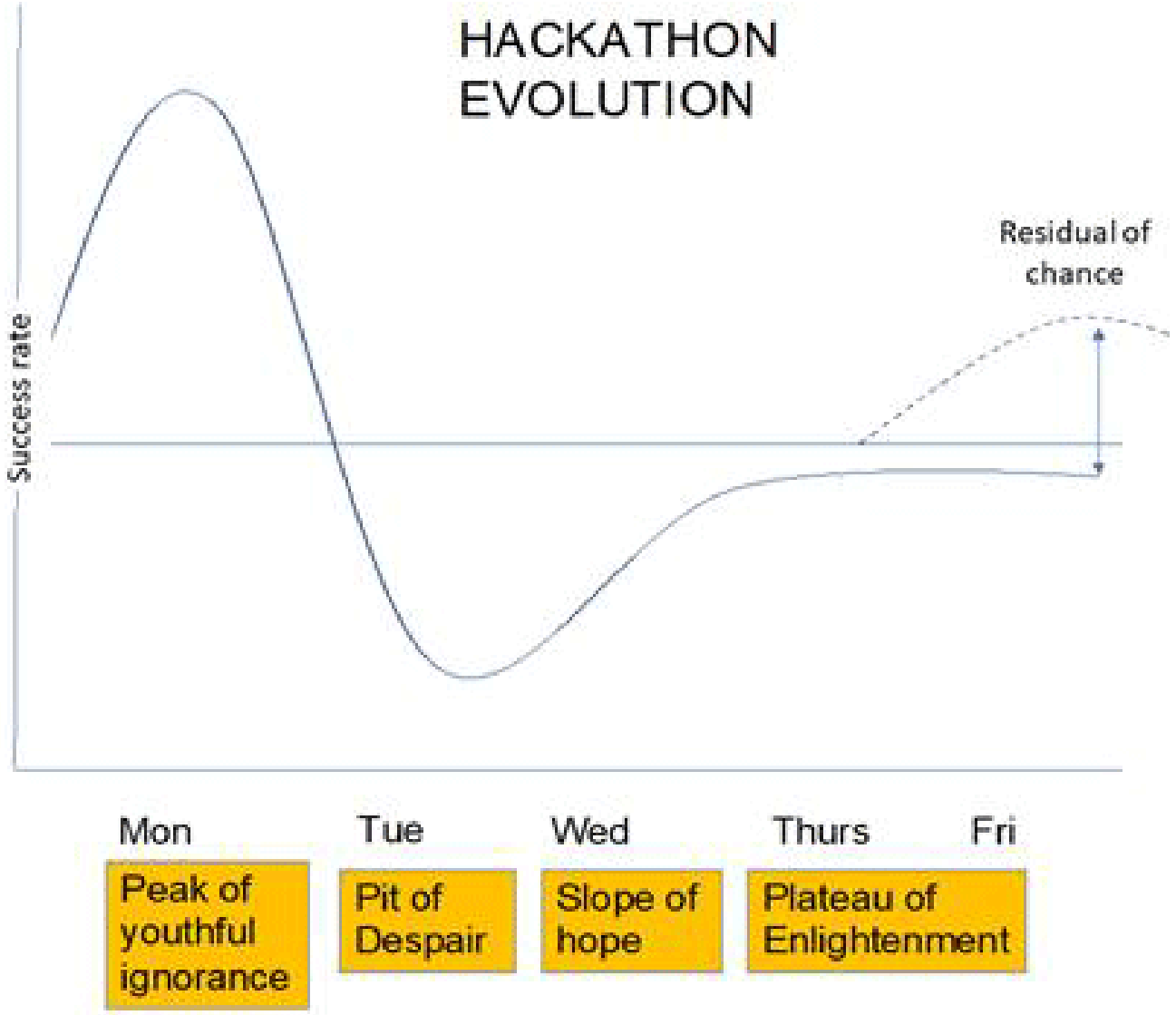
量子技術正以驚人的速度發展，預示著我們即將進入量子計算的時代。在這個過程中，量子電路模擬成為一個關鍵工具，它在量子硬體和軟體的開發中扮演著重要的角色，特別是在處理量子程式的編寫和驗證方面。傳統電腦的強模擬能夠獲得完整的量子狀態信息。這使得傳統電腦在構建量子系統方面變得不可或缺，尤其是在當前噪聲較多的中等規模量子（NISQ）時代。

量子近似優化算法（QAOA）是一種常用的量子算法，用於通過近似解來解決組合優化問題。然而，在虛擬量子計算機上執行QAOA對於解決需要大規模量子電路模擬的組合優化問題而言，會遇到模擬速度較慢的問題。團隊使用數學優化來壓縮量子操作，並結合有效的位元操作進一步降低計算複雜性，透過GPU加速最高獲取468倍的加速效果！

Table 1: The elapsed time of 5-level QAOA (unit: second, double).

Qubit	CPU_{Single}	$CPU_{Mutiple}$	CPU_{Cache}	GPU_{Cache}	GPU_{All}
23	29.80	1.28 (23x)	1.28 (63x)	0.24 (120x)	0.06 (**341x**)
24	68.00	3.46 (20x)	3.46 (43x)	0.55 (123x)	0.12 (**382x**)
25	152.52	15.32 (10x)	15.31 (45x)	1.19 (127x)	0.23 (**404x**)
26	330.69	33.83 (10x)	33.83 (56x)	2.60 (126x)	0.56 (**417x**)
27	712.26	72.66 (10x)	72.66 (54x)	5.59 (127x)	1.08 (**427x**)
28	1556.87	156.52 (10x)	156.52 (54x)	11.96 (130x)	2.17 (**445x**)
29	3325.55	335.09 (10x)	335.09 (49x)	25.73 (129x)	4.45 (**451x**)
30	7226.46	718.33 (10x)	718.33 (47x)	55.20 (130x)	9.22 (**468x**)

更多資訊請看：https://github.com/nqobu/nvidia/raw/main/20231207/Team02.pdf



This article highlights the Oak Ridge Leadership Compute Facilitys GPU Hackathon
https://www.computer.org/csdl/magazine/cs/2018/04/mcs2018040095/13rRUxYIN88

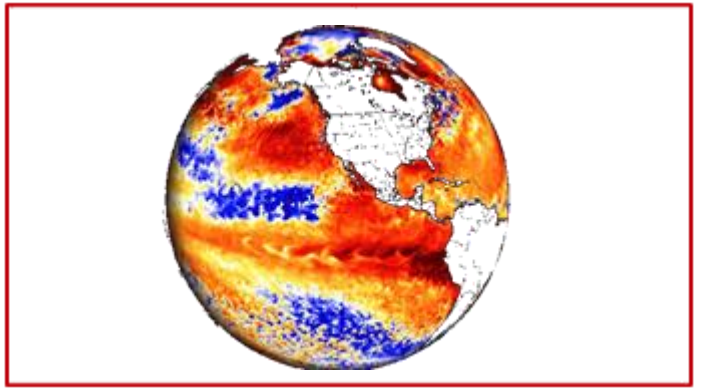
Celebrating Gordon Bell Finalists

Five Gordon Bell Finalists Use the NVIDIA Accelerated Platform for Science at Scale

MULTI-GPU MOLECULAR DYNAMICS
Giuseppe Barca, U. Melbourne

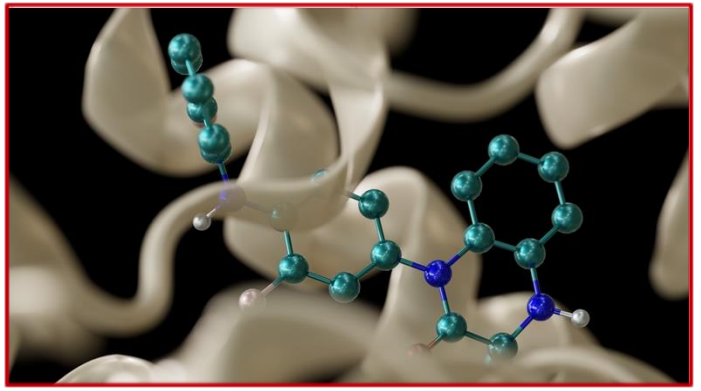
GWAS FOR GENETIC EPISTASIS
David Keyes, KAUST

EMULATION OF GLOBAL ERA5
David Keyes, KAUST

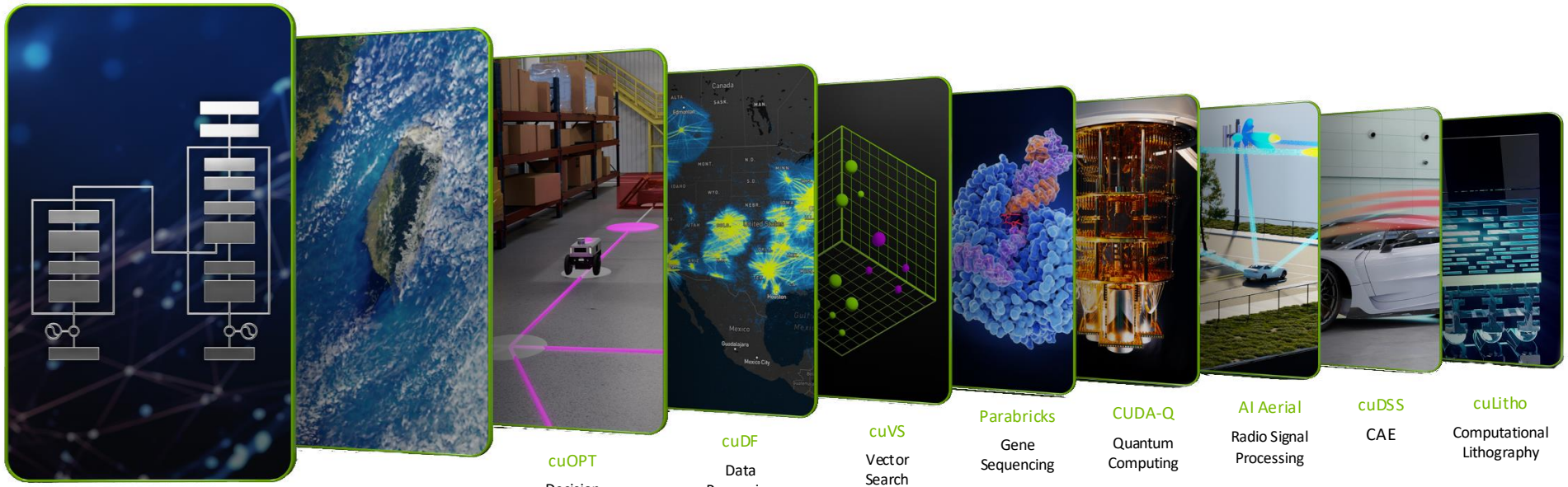


DL FOR TRAINING AND INFERENCE
Abhinav Bhatele, U. Maryland

PROTEIN DESIGN
Arvind Ramanathan, ANL

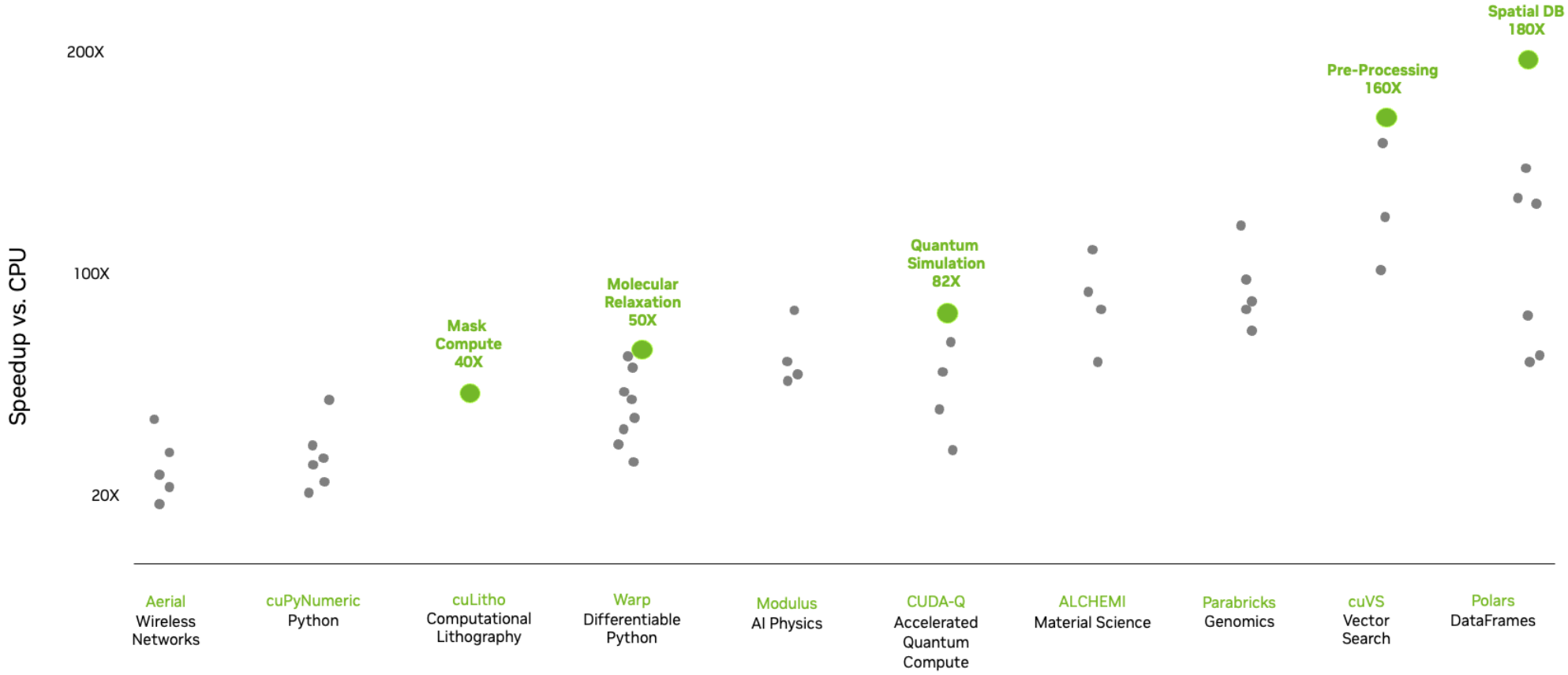


CUDA-X Libraries Accelerate Every Industry



Accelerating Domain Specific Libraries with CUDA-X

Increasing Performance for Hopper GPUs



Super Computer 2024

https://www.nvidia.com/en-us/events/supercomputing/


Thank You
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