# 2019 ISC Student Cluster Competition


Chun-chieh, Chuang
Hsien-ting, Hsieh
Chun-wei, Yang

Cheng-Yu, Huang
Zhong-wei, Hsu
Yen-fu, Liu

Coaches:

Prof. Chi-Chuan, Hwang

Chao-Chin, Li

# 一、官方資料-比賽軟體

| 比賽軟體 | 軟體簡介 |
| --- | --- |
| HPCC | 效能測試軟體，<br>衡量叢集電腦的各種計算能力 |
| HPCG | |
| HPL | |
| OpenFOAM | 計算及模擬流體力學軟體 |
| CP2K | 量子化學計算軟體 |
| Swift | 太空物理計算軟體 |
| Pennant(神秘題) | 2D建模軟體 |
| AI-task(Tensorflow) | 調校模型，依據提供的資料來測試訓練模型的準確度 |

# 二、參與隊伍含設備- 國立成功大學

| **NCKU - 1** | | Amount |
|---|---|---|
| Motherbord | Gigabyte X299-WU8 | 1 |
| CPU | Intel® Core™ i9-9900X | 1 |
| Memory | G.SKILL RGB DDR4-3200 16G | 8 |
| SSD | Intel 760P 2TB/M.2 PCIe | 1 |
| HDD | HGST 10TB | 2 |
| GPU | MSI RTX2080Ti SEA HAWK X 11G | 3 |
| Network | Mellanox Technologies MT27800 Family [ConnectX-5] | 1 |
| Case | ThermalTake Level 20 XT | 1 |
| Power Supply - 1 | Antec 1300W | 1 |
| Power Supply - 2 | SilverStone 1500W | 1 |

| **NCKU - 2** | | Amount |
|---|---|---|
| Motherbord | Gigabyte X299-WU8 | 1 |
| CPU | Intel® Core™ i9-9900X | 1 |
| Memory | G.SKILL DDR4-3200 16G | 8 |
| SSD | Samsung 970 PRO NVMe 1TB/M.2 PCIe | 1 |
| HDD | HGST 10TB | 1 |
| GPU | MSI RTX2080Ti SEA HAWK X 11G | 3 |
| Network | Mellanox Technologies MT27800 Family [ConnectX-5] | 1 |
| Case | ThermalTake Level 20 XT | 1 |
| Power Supply - 1 | Antec 1300W | 1 |
| Power Supply - 2 | SilverStone 1500W | 1 |

# 三、自組電腦的特色

- 每一節點有三張GPU及一個CPU配合128GB的記憶體
- 利用一體成型式消費者型水冷GPU以及渦輪風扇來使GPU降溫
- CPU、記憶體超頻
- GPU核心及記憶體超頻
- 五彩繽紛的RGB風扇、記憶體
- 相較其他隊伍的運算伺服器，我們的花費相當少，估算約為4~5張Nvidia Tesla V100的價錢
- 無使用交換器，使用Infiniband EDR 100GB/s 對接兩節點

# 四、各軟體比賽結果 - AI

| | |
|---|---|
| 使用變數量 | 16 |
| Batch | 16 |
| 學習率 | 0.0001 |
| 訓練Epoches | 200 |

**AI task名次:**

1. ETH Zurich
2. **NCKU**
3. NTU

訓練後使用Evaluation測試集結果: 約79%的IoU

變數說明參考連結: https://github.com/hpcac/ISC19-SCC

# 四、各軟體比賽結果 - HPL

```
CLK=
Per-Process Host Memory Estimate: 13.57 GB (MAX) 13.46 GB (MIN)
Per-Process Host Memory Estimate: 13.46 GB (MAX) 13.39 GB (MIN)
Per-Process Host Memory Estimate: 13.77 GB (MAX) 13.61 GB (MIN)
================================================================================
T/V                N    NB     P     Q               Time                 Gflops
--------------------------------------------------------------------------------
WR03C2L2      100000   256     2     3             205.52             3.244e+03
--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=        5.7842403 ...... PASSED

--
================================================================================
T/V                N    NB     P     Q               Time                 Gflops
--------------------------------------------------------------------------------
WR03C2L2      100000   128     2     3             206.45             3.229e+03
--------------------------------------------------------------------------------
||Ax-b||_oo/(eps*(||A||_oo*||x||_oo+||b||_oo)*N)=       10.4095105 ...... PASSED
```

# 四、各軟體比賽結果 - HPCG

```
Completed Benchmarking Phase... elapsed time: 1852.1 seconds
2019-06-17 22:48:48.797

Number of CG sets:      1248
Iterations per set:     50
scaled res mean:        9.678354e-04
scaled res variance:    1.846129e-39

Total Time: 1.852093e+03 sec
Setup        Overhead: 4.66%
Optimization Overhead: 0.73%
Convergence  Overhead: 0.00%

2x3x1 process grid
256x256x128 local domain
SpMV  =  512.0 GF (3225.1 GB/s Effective)   85.3 GF_per ( 537.5 GB/s Effective)
SymGS =  688.6 GF (5314.9 GB/s Effective)  114.8 GF_per ( 885.8 GB/s Effective)
total =  631.4 GF (4788.2 GB/s Effective)  105.2 GF_per ( 798.0 GB/s Effective)
final =  597.8 GF (4533.4 GB/s Effective)   99.6 GF_per ( 755.6 GB/s Effective)
```

# 四、各軟體比賽結果 - Swift

| # Step | Time | Scale-factor | Redshift | Time-step | Time-bins | | Updates | g-Updates | s-Updates | Wall-clock time [ms] | Props |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1.682968e-02 | 0.9090909 | 0.1000000 | 0.000000e+00 | 1 | 56 | 172460421 | 172460421 | 0 | 87713.938 | 11 |
| 1 | 1.682972e-02 | 0.9090935 | 0.0999968 | 4.148863e-08 | 41 | 41 | 189 | 189 | 0 | 5569.096 | 1 |
| 2 | 1.682976e-02 | 0.9090962 | 0.0999936 | 4.148863e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63054.293 | 0 |
| 3 | 1.682980e-02 | 0.9090988 | 0.0999904 | 4.148863e-08 | 41 | 41 | 216 | 216 | 0 | 5714.053 | 1 |
| 4 | 1.682984e-02 | 0.9091015 | 0.0999872 | 4.148863e-08 | 41 | 43 | 172460421 | 172460421 | 0 | 63058.582 | 0 |
| 5 | 1.682988e-02 | 0.9091041 | 0.0999840 | 4.148863e-08 | 41 | 41 | 270 | 270 | 0 | 5772.222 | 1 |
| 6 | 1.682993e-02 | 0.9091068 | 0.0999808 | 4.148863e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63265.680 | 0 |
| 7 | 1.682997e-02 | 0.9091094 | 0.0999776 | 4.148926e-08 | 41 | 41 | 351 | 351 | 0 | 5810.469 | 1 |
| 8 | 1.683001e-02 | 0.9091121 | 0.0999744 | 4.148893e-08 | 41 | 44 | 172460421 | 172460421 | 0 | 63401.164 | 0 |
| 9 | 1.683005e-02 | 0.9091147 | 0.0999712 | 4.148893e-08 | 41 | 41 | 378 | 378 | 0 | 5731.241 | 1 |
| 10 | 1.683009e-02 | 0.9091173 | 0.0999680 | 4.148896e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63423.324 | 0 |
| 11 | 1.683013e-02 | 0.9091200 | 0.0999648 | 4.148908e-08 | 41 | 41 | 513 | 513 | 0 | 5807.180 | 1 |
| 12 | 1.683017e-02 | 0.9091226 | 0.0999616 | 4.148908e-08 | 41 | 43 | 172460421 | 172460421 | 0 | 63454.508 | 0 |
| 13 | 1.683022e-02 | 0.9091253 | 0.0999584 | 4.148908e-08 | 41 | 41 | 783 | 783 | 0 | 5812.768 | 1 |
| 14 | 1.683026e-02 | 0.9091279 | 0.0999552 | 4.148922e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63456.105 | 0 |
| 15 | 1.683030e-02 | 0.9091306 | 0.0999520 | 4.148923e-08 | 41 | 41 | 837 | 837 | 0 | 5803.502 | 1 |
| 16 | 1.683034e-02 | 0.9091332 | 0.0999488 | 4.148923e-08 | 41 | 45 | 172460421 | 172460421 | 0 | 63665.836 | 0 |
| 17 | 1.683038e-02 | 0.9091359 | 0.0999456 | 4.148933e-08 | 41 | 41 | 864 | 864 | 0 | 5814.684 | 1 |
| 18 | 1.683042e-02 | 0.9091385 | 0.0999424 | 4.148938e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63609.363 | 0 |
| 19 | 1.683046e-02 | 0.9091411 | 0.0999392 | 4.148938e-08 | 41 | 41 | 918 | 918 | 0 | 5850.693 | 1 |
| 20 | 1.683051e-02 | 0.9091438 | 0.0999360 | 4.148943e-08 | 41 | 43 | 172460421 | 172460421 | 0 | 63598.754 | 0 |
| 21 | 1.683055e-02 | 0.9091464 | 0.0999328 | 4.148953e-08 | 41 | 41 | 837 | 837 | 0 | 5799.169 | 1 |
| 22 | 1.683059e-02 | 0.9091491 | 0.0999296 | 4.148953e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63565.566 | 0 |
| 23 | 1.683063e-02 | 0.9091517 | 0.0999264 | 4.148954e-08 | 41 | 41 | 864 | 864 | 0 | 5947.379 | 1 |
| 24 | 1.683067e-02 | 0.9091544 | 0.0999232 | 4.148969e-08 | 41 | 44 | 172460421 | 172460421 | 0 | 63674.855 | 0 |
| 25 | 1.683071e-02 | 0.9091570 | 0.0999200 | 4.148969e-08 | 41 | 41 | 783 | 783 | 0 | 5844.495 | 1 |
| 26 | 1.683076e-02 | 0.9091597 | 0.0999168 | 4.148969e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63781.738 | 0 |
| 27 | 1.683080e-02 | 0.9091623 | 0.0999136 | 4.148980e-08 | 41 | 41 | 729 | 729 | 0 | 5834.366 | 1 |
| 28 | 1.683084e-02 | 0.9091649 | 0.0999104 | 4.148984e-08 | 41 | 43 | 172460421 | 172460421 | 0 | 63547.961 | 0 |
| 29 | 1.683088e-02 | 0.9091676 | 0.0999072 | 4.148984e-08 | 41 | 41 | 621 | 621 | 0 | 5810.256 | 1 |
| 30 | 1.683092e-02 | 0.9091702 | 0.0999040 | 4.148991e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63643.668 | 0 |
| 31 | 1.683096e-02 | 0.9091729 | 0.0999008 | 4.148999e-08 | 41 | 41 | 567 | 567 | 0 | 5768.729 | 1 |
| 32 | 1.683100e-02 | 0.9091755 | 0.0998976 | 4.148999e-08 | 41 | 46 | 172460421 | 172460421 | 0 | 63754.270 | 0 |
| 33 | 1.683105e-02 | 0.9091782 | 0.0998944 | 4.149002e-08 | 41 | 41 | 513 | 513 | 0 | 5777.681 | 1 |
| 34 | 1.683109e-02 | 0.9091808 | 0.0998912 | 4.149014e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63631.484 | 0 |
| 35 | 1.683113e-02 | 0.9091835 | 0.0998880 | 4.149014e-08 | 41 | 41 | 351 | 351 | 0 | 5807.415 | 1 |
| 36 | 1.683117e-02 | 0.9091861 | 0.0998848 | 4.149014e-08 | 41 | 43 | 172460421 | 172460421 | 0 | 63666.906 | 0 |
| 37 | 1.683121e-02 | 0.9091887 | 0.0998816 | 4.149028e-08 | 41 | 41 | 189 | 189 | 0 | 5859.421 | 1 |
| 38 | 1.683125e-02 | 0.9091914 | 0.0998784 | 4.149029e-08 | 41 | 42 | 172460421 | 172460421 | 0 | 63762.715 | 0 |
| 39 | 1.683129e-02 | 0.9091940 | 0.0998752 | 4.149029e-08 | 41 | 41 | 135 | 135 | 0 | 5784.985 | 1 |
| 40 | 1.683134e-02 | 0.9091967 | 0.0998720 | 4.149039e-08 | 41 | 44 | 172460421 | 172460421 | 0 | 63730.312 | 0 |
| 41 | 1.683138e-02 | 0.9091993 | 0.0998688 | 4.149044e-08 | 41 | 41 | 216 | 216 | 0 | 5846.027 | 1 |

# 四、各軟體比賽結果 - Pennant

```
Run complete
cycle = 115921,          cstop = 999999
time  =   1.100000e+01, tstop =   1.100000e+01

**********************************
hydro cycle run time=   7.841887e+03
**********************************
Energy check:  total energy  =   9.424778e-01
(internal =   6.131684e-01, kinetic =   3.293094e-01)
```

# 四、各軟體比賽結果 - CP2K

| SUBROUTINE | CALLS | ASD | SELF TIME | | TOTAL TIME | |
|---|---|---|---|---|---|---|
| | MAXIMUM | | AVERAGE | MAXIMUM | AVERAGE | MAXIMUM |
| CP2K | 1 | 1.0 | 0.021 | 0.024 | 1242.214 | 1242.234 |
| qs_mol_dyn_low | 1 | 2.0 | 257.192 | 280.916 | 1234.606 | 1236.060 |
| velocity_verlet | 50 | 3.0 | 0.160 | 0.163 | 919.447 | 919.507 |
| qmmm_forces | 51 | 4.0 | 0.159 | 0.173 | 504.631 | 504.648 |
| deriv_dftb_qmmm_matrix | 51 | 5.0 | 0.156 | 0.167 | 504.373 | 504.379 |
| build_mm_pot | 59262 | 6.0 | 364.976 | 378.664 | 364.976 | 378.664 |
| build_mm_dpot | 29631 | 6.0 | 308.676 | 313.041 | 308.676 | 313.041 |
| qs_forces | 51 | 4.0 | 0.010 | 0.011 | 241.938 | 241.943 |
| qs_energies | 51 | 5.0 | 0.002 | 0.002 | 240.914 | 240.938 |
| scf_env_do_scf | 51 | 6.0 | 0.001 | 0.010 | 228.101 | 228.273 |
| scf_env_do_scf_inner_loop | 515 | 6.9 | 0.016 | 0.062 | 228.099 | 228.262 |
| qs_scf_new_mos | 515 | 7.9 | 0.008 | 0.008 | 225.881 | 225.932 |
| qmmm_el_coupling | 51 | 4.0 | 0.001 | 0.001 | 183.083 | 189.851 |
| build_dftb_qmmm_matrix | 51 | 5.0 | 0.078 | 0.084 | 183.080 | 189.848 |
| eigensolver | 515 | 8.9 | 0.028 | 0.040 | 181.994 | 182.037 |
| cp_fm_syevd | 515 | 9.9 | 0.004 | 0.004 | 154.483 | 154.685 |
| cp_fm_syevd_base | 515 | 10.9 | 154.478 | 154.681 | 154.478 | 154.681 |
| fist_calc_energy_force | 51 | 4.0 | 0.333 | 0.349 | 43.470 | 112.622 |
| mp_sum_d | 3932 | 8.9 | 25.737 | 89.813 | 25.737 | 89.813 |
| qs_diis_b_step | 464 | 8.9 | 0.025 | 0.026 | 34.660 | 34.703 |
| cp_fm_cholesky_restore | 1545 | 9.9 | 24.981 | 25.755 | 24.981 | 25.755 |

# 四、各軟體比賽結果 - OpenFOAM

```
Time = 400

smoothSolver:  Solving for Ux, Initial residual = 6.66479e-05,
smoothSolver:  Solving for Uy, Initial residual = 0.00122214,
smoothSolver:  Solving for Uz, Initial residual = 0.00128758,
 Final residual = 2.72907e-06,
Final residual = 5.09912e-05,
Final residual = 5.37763e-05,
```

```
GAMG:  Solving for p, Initial residual = 0.0023472, Final residual = 0.00022562, No Iterations 2
time step continuity errors : sum local = 2.09601e-05, global = 8.70583e-08, cumulative = 0.00199659
smoothSolver:  Solving for nuTilda, Initial residual = 9.32826e-05, Final residual = 8.98225e-06, No Iterations 2
```

```
ExecutionTime = 5224.2 s  ClockTime = 5330 s
```