



# TSUBAME Grand Challenge program



## Large Scale Applications on TSUBAME2.5

### TSUBAME Grand Challenge program

TSUBAME Grand Challenge program is only chance to use all nodes of TSUBAME2.5 exclusively, because TSUBAME2.5 is shared by thousands of users.

There are two categories:

#### Category A

The large scale application aims high peak-performance.

All of TSUBAME2.5 nodes are available.

#### Category B

The large scale application aims scientifically meaningful results.

A large portion (1/3) of TSUBAME2.5 is available.

We started this program since FY2011, and keep on carrying out twice in each year.

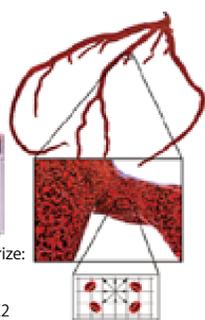
Table Number of Adopted Projects in the TSUBAME Grand-Challenge Program

| Category | FY2014 |            | FY2013 |      | FY2012 |      | FY2011 |      | Total |    |
|----------|--------|------------|--------|------|--------|------|--------|------|-------|----|
|          | Fall   | First Half | Fall   | Spr. | Fall   | Spr. | Fall   | Spr. |       |    |
| A        | 1      | —          | 2      | 0    | 1      | 2    | 2      | 3    | 4     | 15 |
| B        | 2      | 2          | 0      | 1    | 1      | 0    | 0      | 2    | -     | 8  |
| Total    | 3      | 2          | 2      | 1    | 2      | 2    | 2      | 5    | 4     | 23 |

Under this program, we have adopted total 23 fruitful projects, some of which were awarded prizes as below.



2011 ACM Gordon Bell Prize: Special Achievements in Scalability and Time-to-Solution "Peta-scale Phase-Field Simulation for Dendritic Solidification on the TSUBAME 2.0 Supercomputer"



2011 Graph500 Challenge on TSUBAME 2.0

2011 ACM Gordon Bell Prize: Honorable Mention Large scale biofluidics simulations on TSUBAME2

### Global Atmosphere Simulation on GPU supercomputer using OpenACC

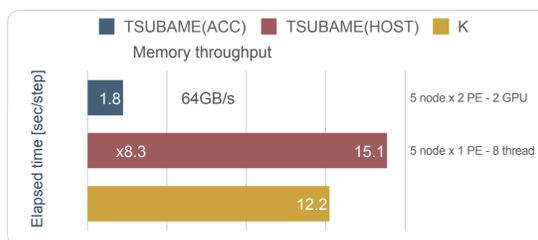
Hisashi Yashiro\*, Akira Naruse\*\*, Ryuji Yoshida\*, Hirofumi Tomita\*  
\*RIKEN Advanced Institute for Computational Science, \*\*NVIDIA

• Dynamical core of NICAM (packaged as "NICAM-DC") is used



Nonhydrostatic ICosahedral Atmospheric Model (NICAM)

- Global, ultra-high-resolution, weather & climate model
- Finite-volume method on icosahedral grid system
- A first global sub-km simulation (right figure) was executed in 2013



Advantage of OpenACC

- Small modification, directive-based
- Reduce the time to develop
- Keep from splitting the source code : Only 2000 lines are modified/added to the source code

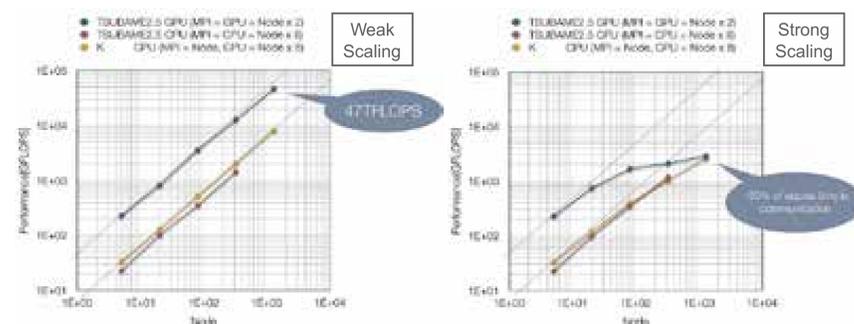
• Performance evaluation on TSUBAME 2.5

: 10 to 2560 GPU (60% of full system)

• J&W (2006) test case was carried out: Not a kernel test, includes communication and file I/O

• We obtained good computational performance

(appropriate for the memory performance of GPU), as well as weak scalability



### Solving the Schrödinger Equations of Some Organic Molecules

Hiroshi Nakatsuji, Hiroyuki Nakashima (Quantum Chemistry Research Institute)

The purpose of "first-principle simulation" is to give a perfect prediction of phenomena. Since the Schrödinger equation is the governing principle of chemistry, one should be able to predict chemical phenomena based on the exact solutions of this equation. Since 2000, Nakatsuji and his colleagues have been successful to formulate a general theory of exactly solving this equation: the free complement (FC) theory combined with the local Schrödinger equation (LSE) method is applicable to any atomic and molecular systems. Recently, we performed the FC-LSE calculations of some simple organic molecules using the superparallel computer TSUBAME in the occasion of Grand Challenge and obtained accurate wave functions and absolute energies satisfying chemical accuracy (kcal/mol). In the calculations, the computational tasks due to the sampling can be equally distributed to each process (core). In fact, the parallel efficiency 111.5 % could be achieved with the test calculation of benzene using 4600 cores of the superparallel computer TSUBAME. The present accurate solutions of the Schrödinger equations of organic molecules are of significant importance in science that provides a basis for future development in theoretical and computational chemistry.

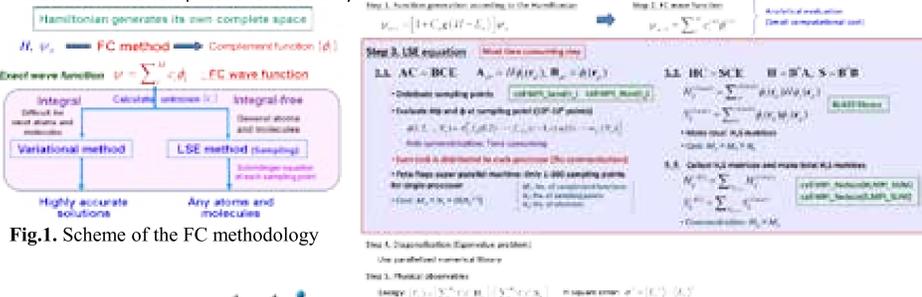


Fig. 1. Scheme of the FC methodology

Fig. 2. Parallel algorithm of the FC-LSE method

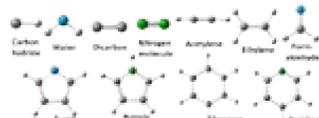


Fig. 3. Some organic molecules to which the FC-LSE method was applied

Table 1. Solving the Schrödinger equations of small organic molecules (Order of the FC method: n=2)

| Molecule                                   | No. of elec. | Dimension n | Energy (a.u.) |                              | $\Delta E = E_{FC-LSE} - E_{Exact}$ (kcal/mol) |
|--|--------------|-------------|---------------|------------------------------|--|
|  |              |             | FC-LSE        | Estimated exact (experiment) |  |
| Carbon hydride (CH)                        | 7            | 1503        | -38.480 41    | -38.479 0                    | -0.88  |
| Water (H <sub>2</sub> O)                   | 10           | 2075        | -76.456 78    | -76.457 8                    | 0.67   |
| Dicarbon (C <sub>2</sub> )                 | 12           | 1976        | -75.923 69    | -75.926 5                    | -0.44  |
| Nitrogen molecule (N <sub>2</sub> )        | 14           | 1121        | -109.542 07   | -109.542 7                   | 0.39   |
| Acetylene (C <sub>2</sub> H <sub>2</sub> ) | 14           | 1709        | -77.333 31    | -77.335 7                    | 1.49   |
| Ethylene (C <sub>2</sub> H <sub>4</sub> )  | 16           | 2628        | -78.577 95    | -78.587 4                    | 5.93   |
| Formaldehyde (H <sub>2</sub> CO)           | 16           | 4083        | -114.505 35   | -114.508 0                   | 1.66   |

Table 2. Test calculations of medium-size organic molecules (Order of the FC method: n=1)

| Molecule                                   | No. of elec. | Dimension n | Energy (a.u.) |                              | $\Delta E = E_{FC-LSE} - E_{Exact}$ (a.u.) |
|--|--------------|-------------|---------------|------------------------------|--|
|  |              |             | FC-LSE        | Estimated exact (experiment) |  |
| Furan (C <sub>4</sub> H <sub>4</sub> O)    | 36           | 161         | -229.860 1    | -230.027                     | 0.167                                      |
| Pyrrrole (C <sub>4</sub> H <sub>3</sub> N) | 36           | 174         | -209.974 3    | -210.173                     | 0.199                                      |
| Benzene (C <sub>6</sub> H <sub>6</sub> )   | 42           | 398         | -232.409 3    | -232.248                     | -0.161                                     |
| Pyridine (C <sub>5</sub> H <sub>5</sub> N) | 42           | 5092*       | -232.195 8*   | -232.195                     | -0.052*                                    |
| Pyridine (C <sub>5</sub> H <sub>5</sub> N) | 42           | 386         | -247.704 1    | (-248.290)                   | 0.586                                      |

\* Large FC order for the carbon atoms

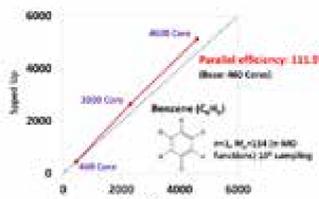
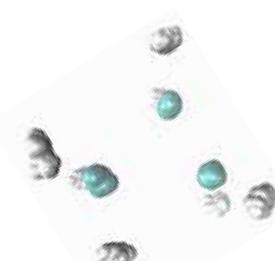


Fig. 4. Timing test with benzene for the parallel efficiency

### Ab Initio Path Integral MD Simulation for Molecular Structure

Tsutomu Kawatsu<sup>a,b</sup>, Masanori Tachikawa<sup>b</sup> / <sup>a</sup>Univ. of Tokyo, <sup>b</sup>Yokohama City Univ.

Ab initio path integral molecular dynamics (PIMD) simulation is performed to obtain geometrical distribution of a protonated cyclopropane.



A partition function is written by classical particles

$$Z = \text{Tr}(e^{-\beta \hat{H}}) = \text{Tr}(e^{-\beta H/P})^P$$

$$= \lim_{P \rightarrow \infty} \prod_{i=1}^P \int \left( \frac{M_i P}{2\pi\beta\hbar^2} \right)^{3P} \int \dots \int dr_1^{(1)} \dots dr_N^{(1)} dr_1^{(2)} \dots dr_N^{(P-1)} \exp(-\beta V_{eff})$$

$$\hat{H} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2M_i} + V_0(r_1 \dots r_N)$$

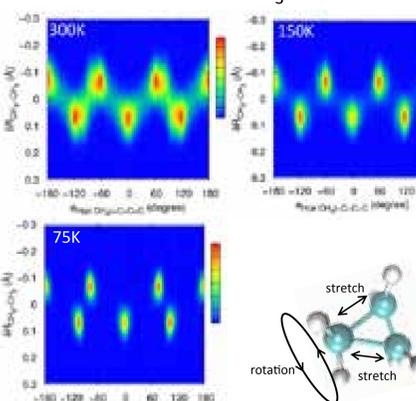
Hamiltonian for N quantum particles

A protonated cyclopropane molecule drawn by N x P classical particles

$$V_{eff} = \sum_{s=1}^P \left[ \sum_{i=1}^N \frac{M_i P}{2\beta^2 \hbar^2} (R_i^{(s)} - R_i^{(s+1)})^2 + \frac{1}{P} V_0(R_1^{(s)} \dots R_N^{(s)}) \right]$$

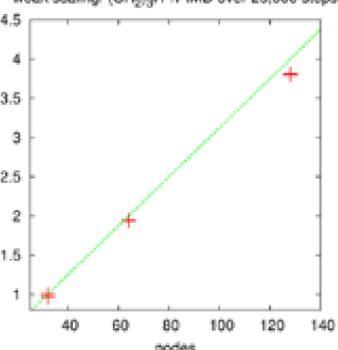
Effective potential for N x P classical particles

Geometrical distribution of C-C bond stretches and CH<sub>3</sub> rotation



Performance in TSUBAME

weak scaling/ (CH<sub>2</sub>)<sub>3</sub>H<sup>+</sup>/PIMD over 26,000 steps



(Single ab initio calculation is performed per node for each step using GAMESS)