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CCS-EPCC Workshop
@ CCS, University of Tsukuba

# Computational Bioscience Utilizing Supercomputers: Performance and Applications

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T2K-Tsukuba, CCS, Univ. Tsukuba
HECToR, EPCC, Univ. Edinburgh

# Outline

1. Performance Benchmarks for First Principle Calculations in Supercomputers (HECToR, T2K-Tsukuba)

2. GPU acceleration for Hartree-Fock (HF) calculation

3. Recent results of Quantum Mechanics/ Molecular Mechanics (QM/MM)

(4. Recent results for Molecular Dynamics)

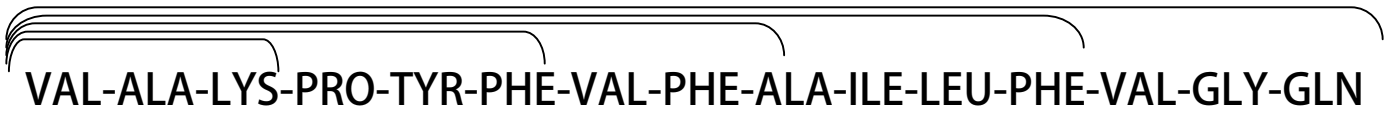
# 1. Performance Benchmarks for First Principle Calculations in Supercomputers

(HECToR, T2K-Tsukuba)

# First Principle Calculations (Quantum Mechanics)

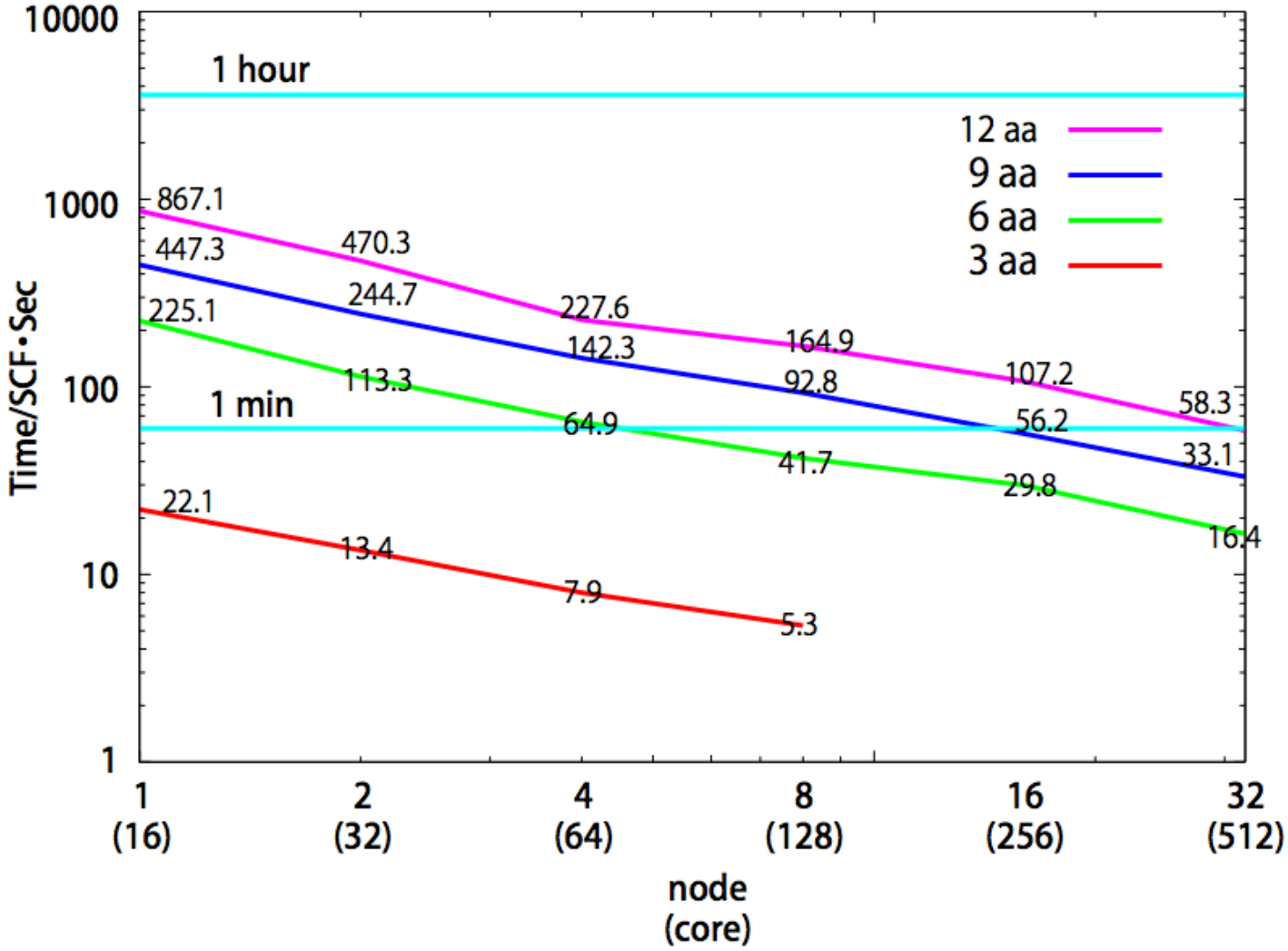
- Method: B3LYP/6-31G* using NWChem(Ver 6.0)
- System: Alpha Helix # amino acids (# basis sets)

  3(388) 6(1011) 9(1421) 12(1888) 15(2228)



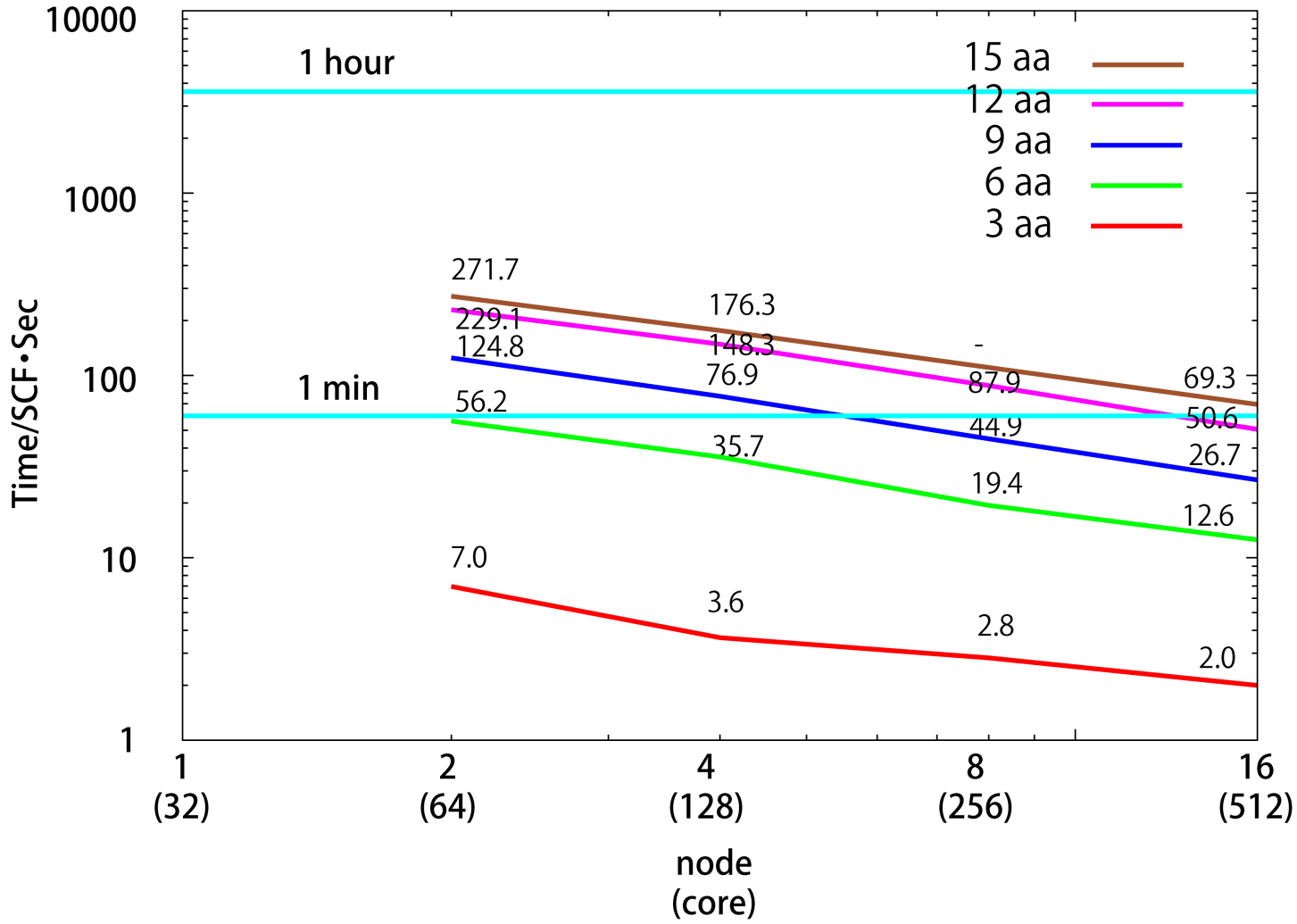
# T2K-Tsukuba

- Opteron 8000 Quad-core x 4 sockets/node (16 core/node)
- 32GB memory/node , Infiniband
- ~95Tflops



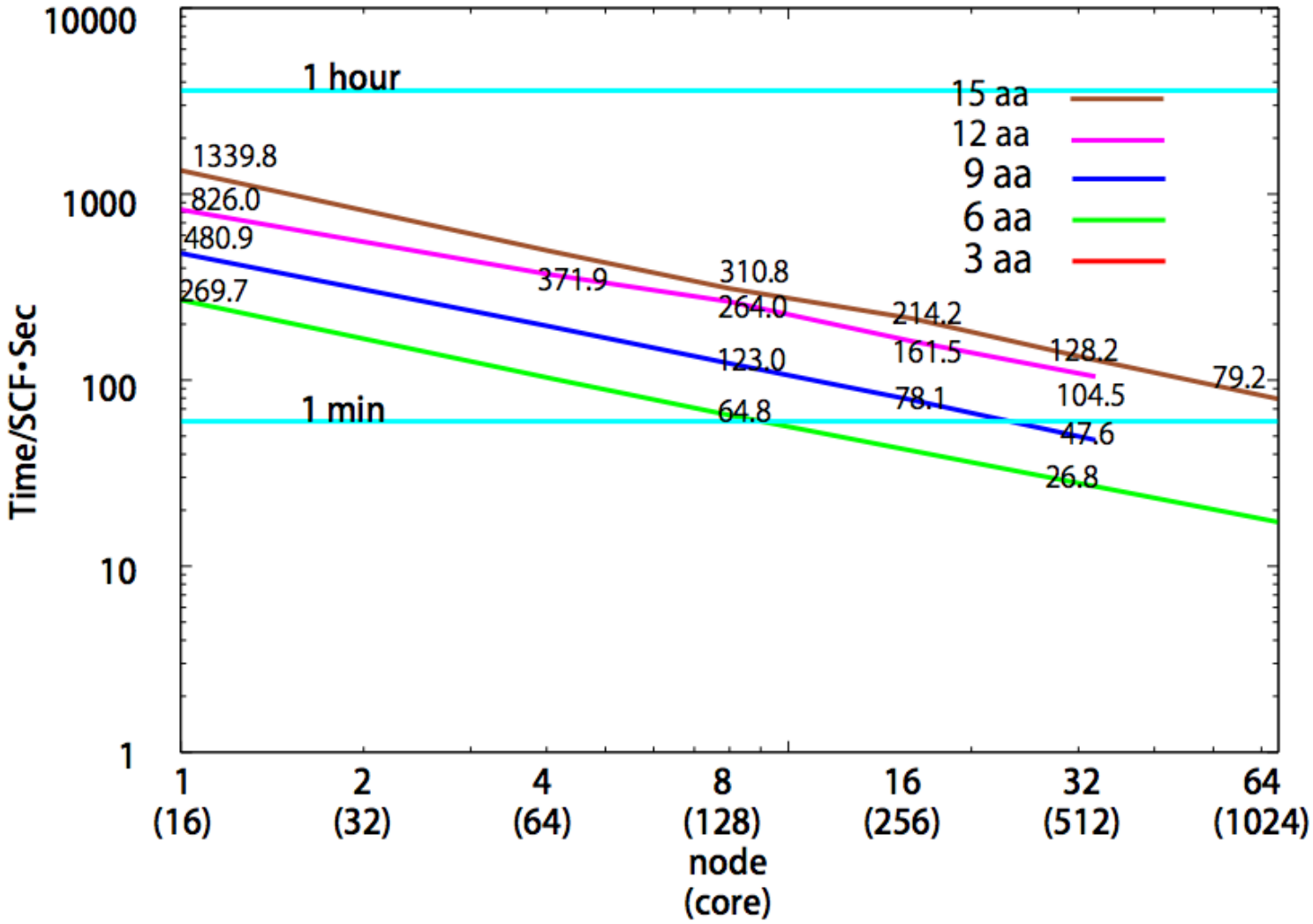
# HECToR Phase3

- Opteron (Interlagos)x 2 sockets/node (32core/node) X 2816 node
- 32GB memory/node
- ~800Tflops



# T2K-Tokyo (HA8000)

- Opteron 8356 Quad-core x 4 sockets/node (16 core/node)
- 32GB memory/node, Myrinet-10G
- Top84 (2011/6)

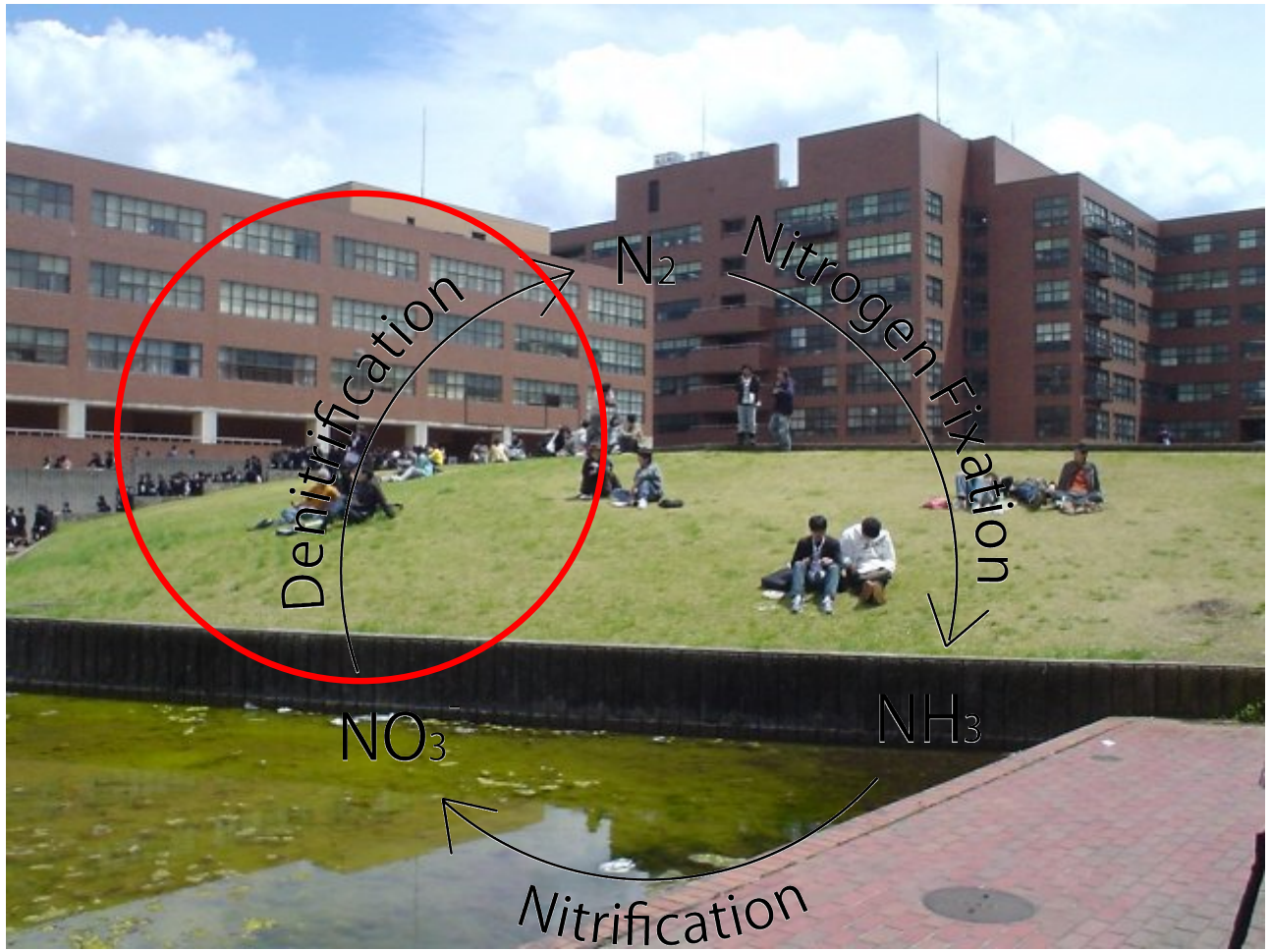


# Comparison at a typical case

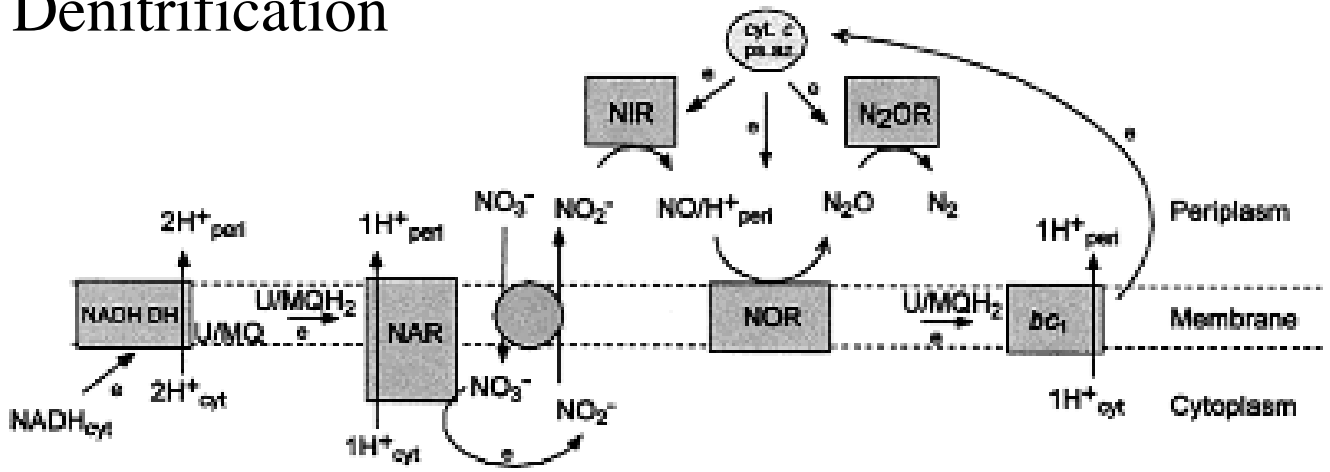
| | 1SCF/s , 12aa | core(node) |
|---|---|---|
| HECToR (Phase3 ) | 87.9 | 256 (8) |
| HECToR (Phase2b) | 105.8 | 256 (~10.6) |
| T2K-Tsukuba | 107.2 | 256 (16) |
| T2K-Tokyo | 161.5 | 256(16) |

# 3. A QM/MM study on a reaction mechanism of nitric oxide reductase (NOR)

# Global Nitrogen Cycle



# Denitrification




$$NO_3^- \xrightarrow{NAR} NO_2^- \xrightarrow{NIR} NO \xrightarrow{NOR} N_2O \xrightarrow{N_2OR} N_2$$

Nitrate reductase (NAR)

$NO_3^- + QH_2 + 2H+ \rightarrow NO_2^- + Q + 2H+ H_2O$

Nitrite Reductase (NIR)

$NO_2^- + 1e^- + 2H^+ \rightarrow NO + H_2O$

Nitric Oxide Reductase (NOR)

$2NO + 2\ e^- + 2H^+ \rightarrow N_2O + H_2O$

Nitrous Oxide Reductase ($N_2OR$)

$N_2O + 2e^- + 2H^+ \rightarrow N_2 + H_2O$

# Nitric oxide reductase (NOR)

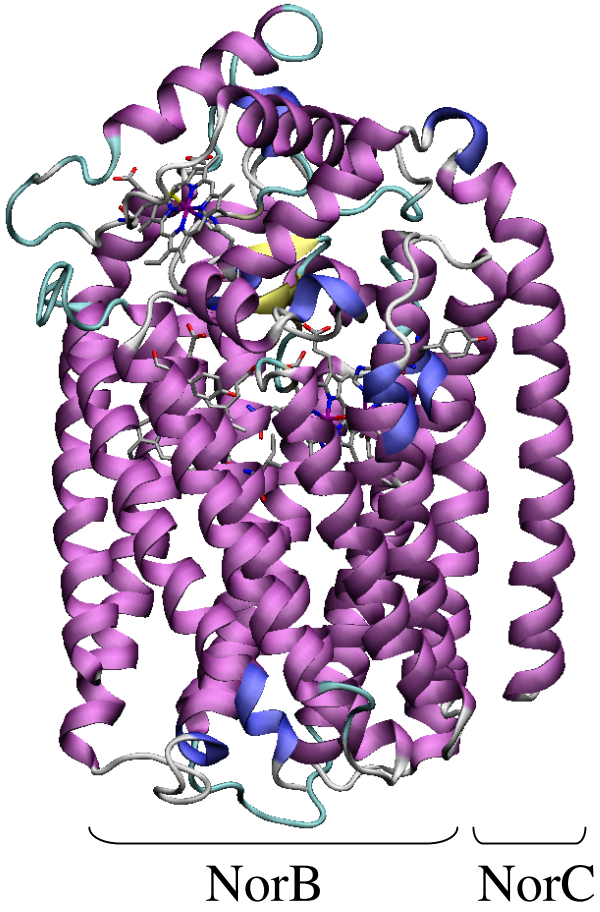
- Reduction of nitric oxide (NO) to nitrous oxide ($N_2O$)
  $2NO + 2\ e^- + 2H^+ \rightarrow N_2O + H_2O$
- Include a N-O bond cleavage and a N-N bond formation
- $N_2O$ is a greenhouse gas

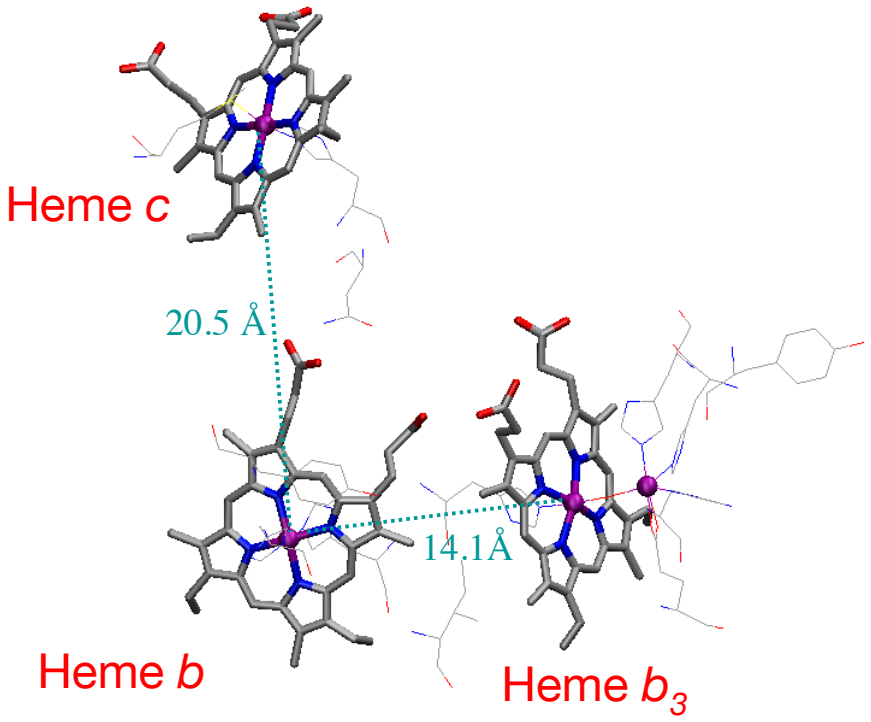
- First x-ray structure was resolved in 2010 [1].
- Many similarities to cytochrome c oxidase (COX)
- D, K-proton pathway is missing in NOR

[1] T. Hino et al, Science 330, 1666(2010)

- 3 reaction mechanisms are proposed.
  (*trans*, *cis*-$Fe_B$, *cis*-heme $_{b3}$)

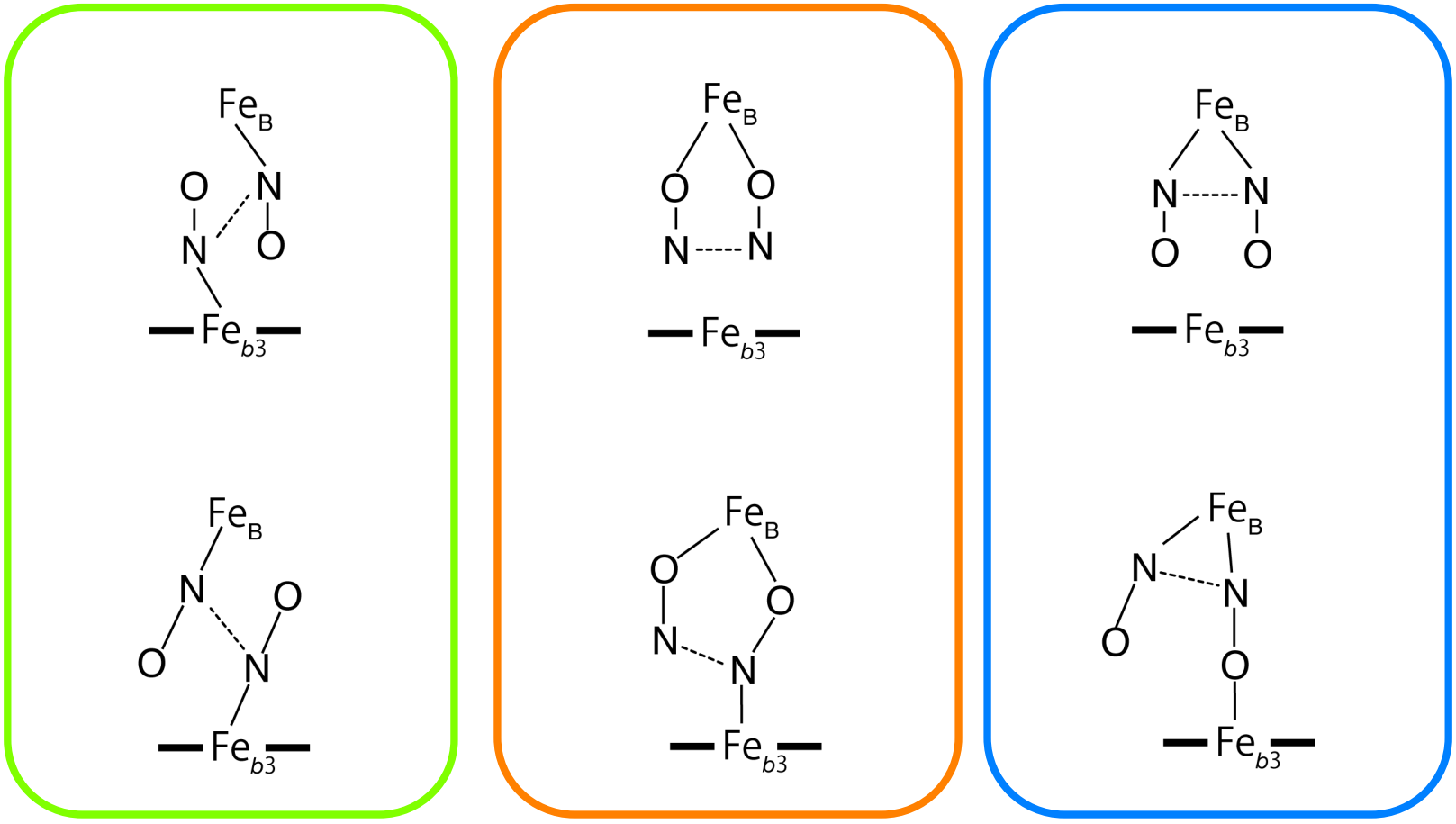
# Structure of NOR [1]




[1] T. Hino et al, Science 330, 1666(2010)

# Proposed reaction mechanisms




*Trans*

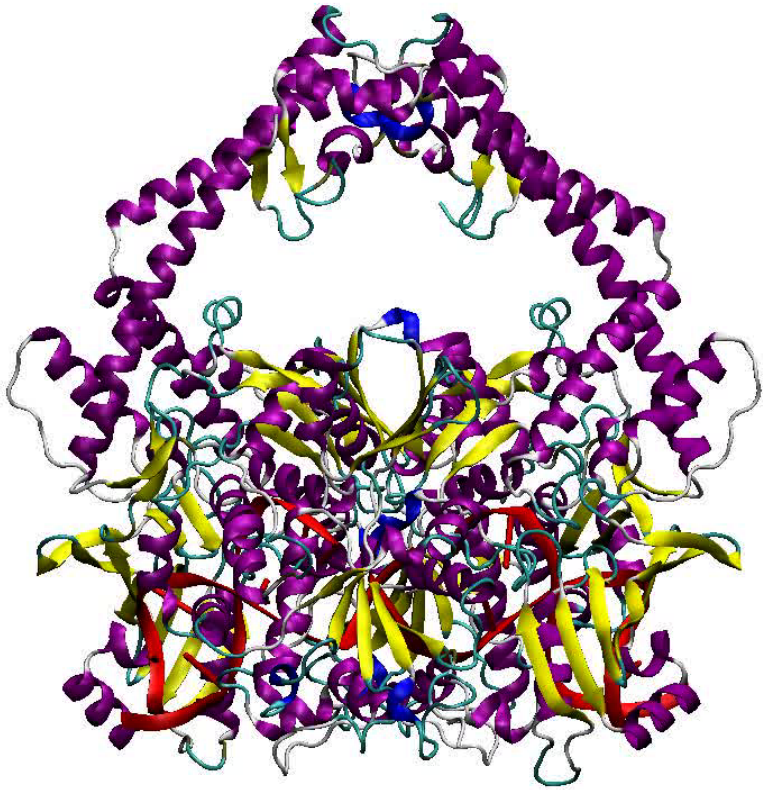
*cis*-heme $_{b3}$

*cis*-FeB

# 3. Recent results for Molecular Dynamics (DNA-Topoisomerase, Prion Protein)

# DNA-Topoisomerase

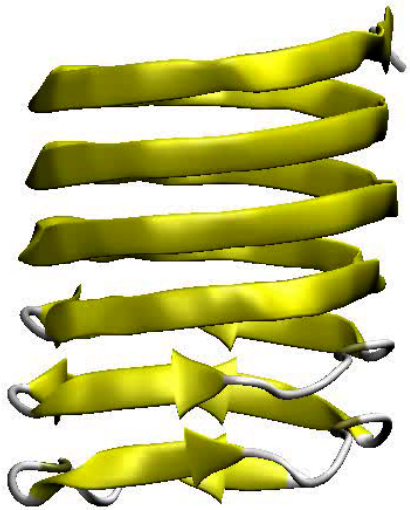
- DNA Topoisomerase: catalyzes interconversions of the different topological forms of DNA
- important drag target for cancer and antibiotical agent



# Prion Protein

Prions are infectious proteins, where self-propagating amyloid conformations of proteins are transmitted.

Prions cause neurodegenerative disease such as bovine spongiform encephalopathy (BSE) and variant Creutzfeldt-Jakob disease (CJD)



Thank you for your attention!

# Group trip @ Mt. Tsukuba 14/3/2012