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@ CCS, University of Tsukuba

Computational Bioscience Utilizing Supercomputers: Performance and Applications

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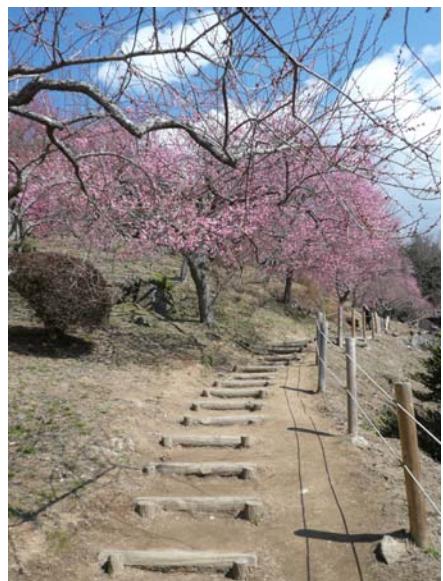
Mitsuhisa Sato (Prof.)



Acknowledgements

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

Group trip @ Mt. Tsukuba 14/3/2012



Outline

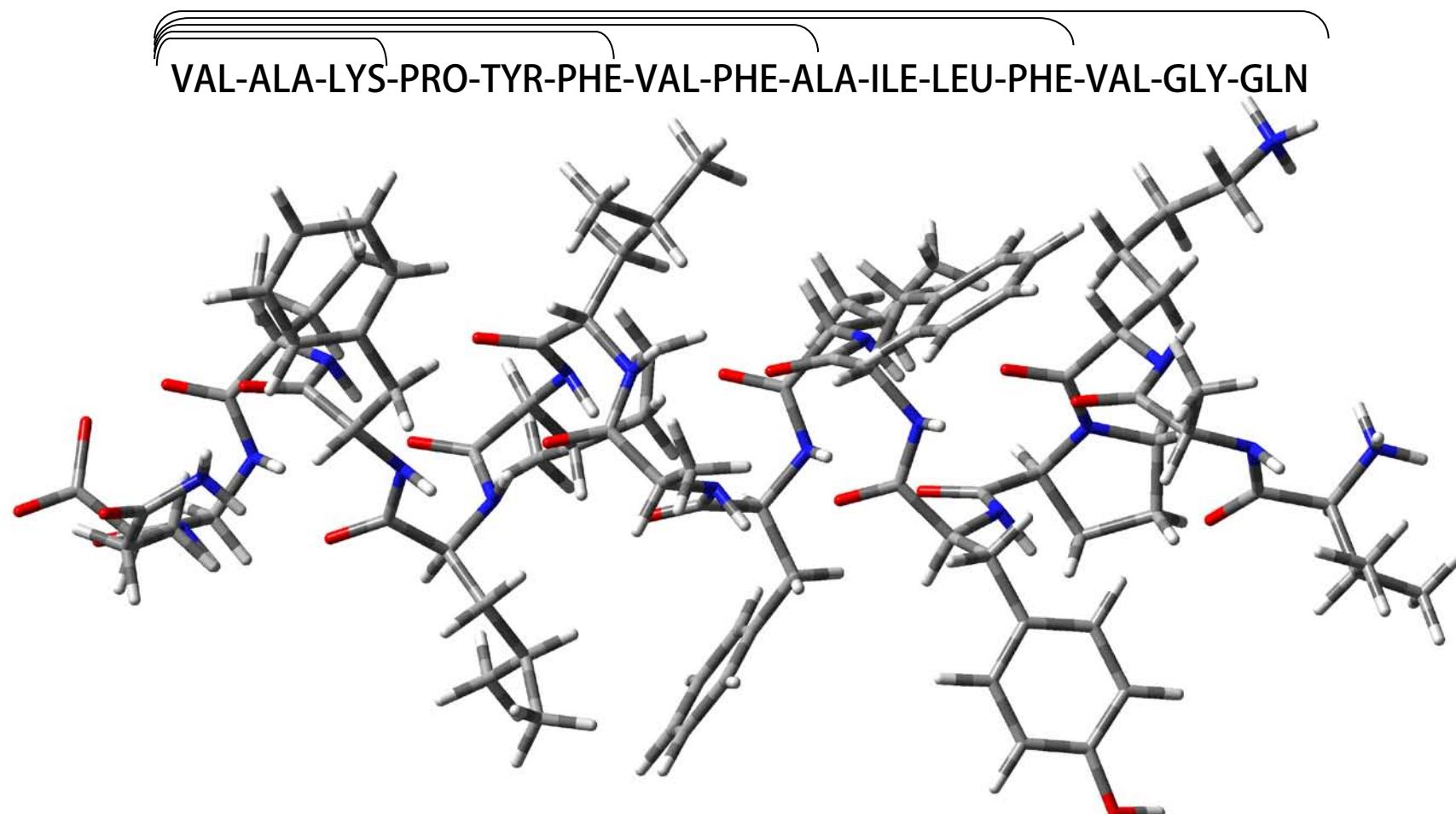
1. Performance Benchmarks for First Principle Calculations in Supercomputers (HECToR, T2K-Tsukuba)
2. A Quantum Mechanics/ Molecular Mechanics (QM/MM) study on a reaction mechanism of nitric oxide reductase (NOR)
3. Recent results for Molecular Dynamics

1. Performance Benchmarks for First Principle Calculations in Supercomputers

(HECToR, T2K-Tsukuba)

First Principle Calculations (Quantum Mechanics)

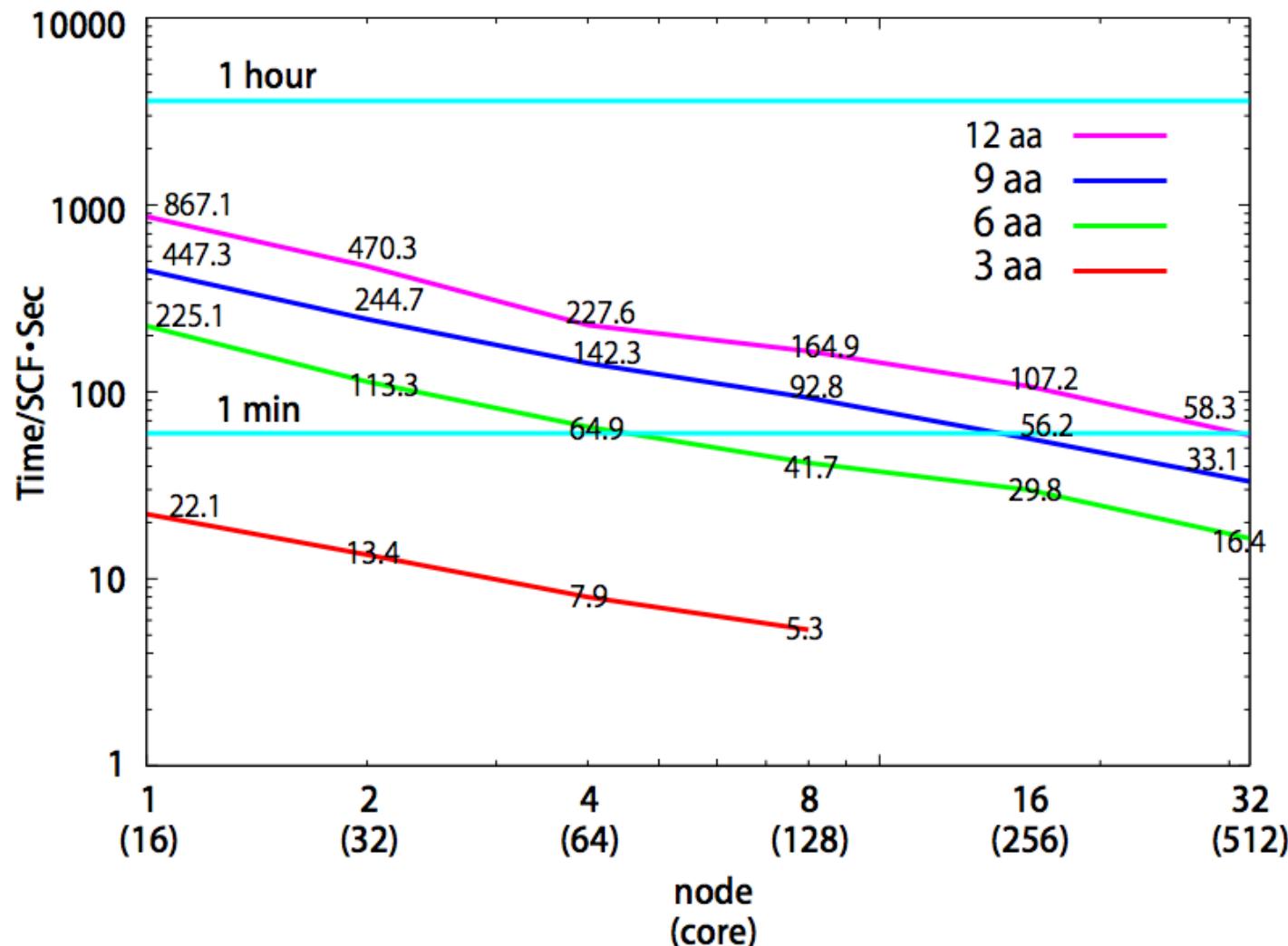
- Method: B3LYP/6-31G* using NWChem(Ver 6.0)
- System: Alpha Helix # amino acids (# basis sets)
3(388) 6(1011) 9(1421) 12(1888) 15(2228)



T2K-Tsukuba



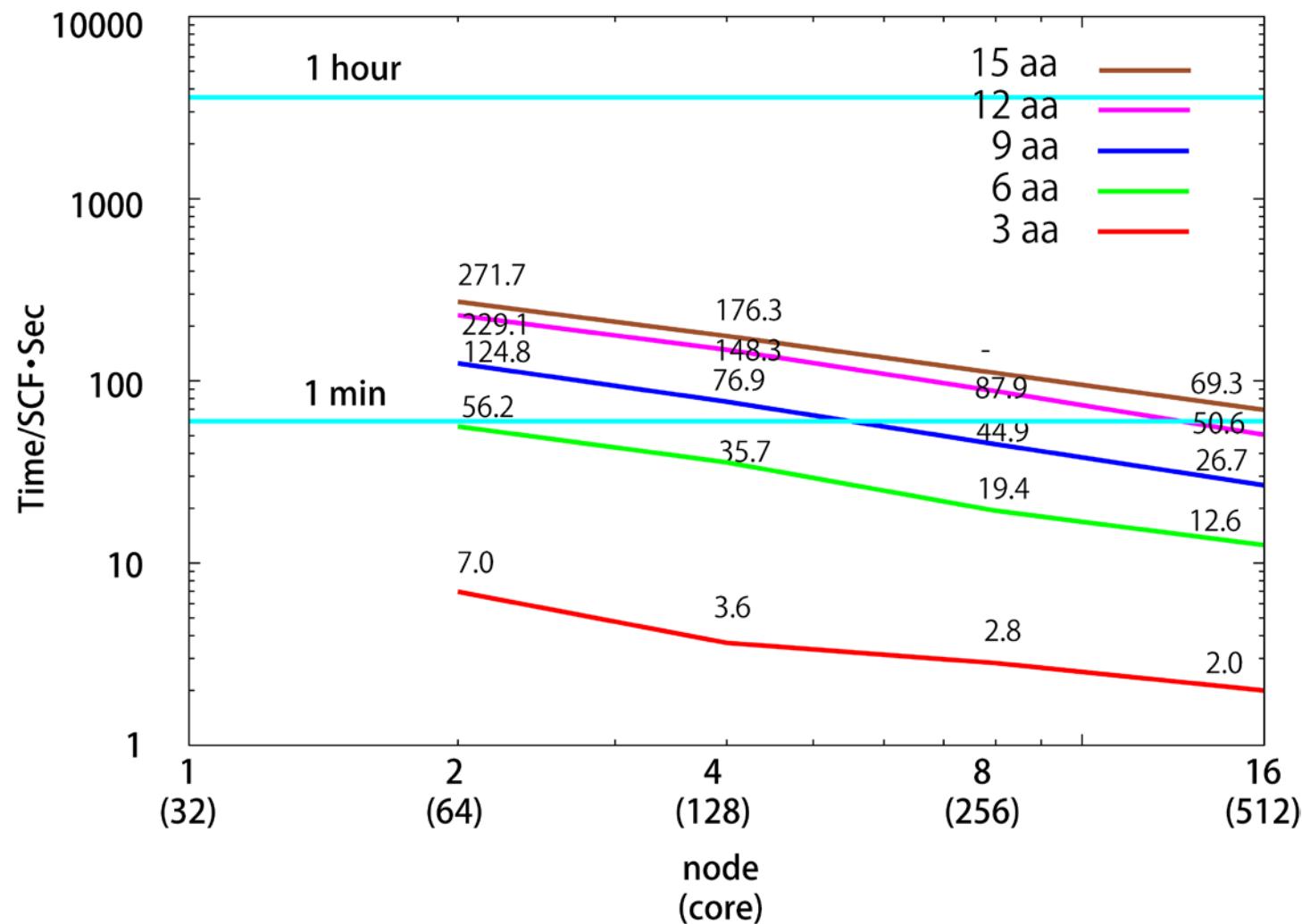
- Opteron 8000 Quad-core x 4 sockets/node (16 core/node)
- 32GB memory/node , Infiniband
- ~95Tflops



HECToR Phase3



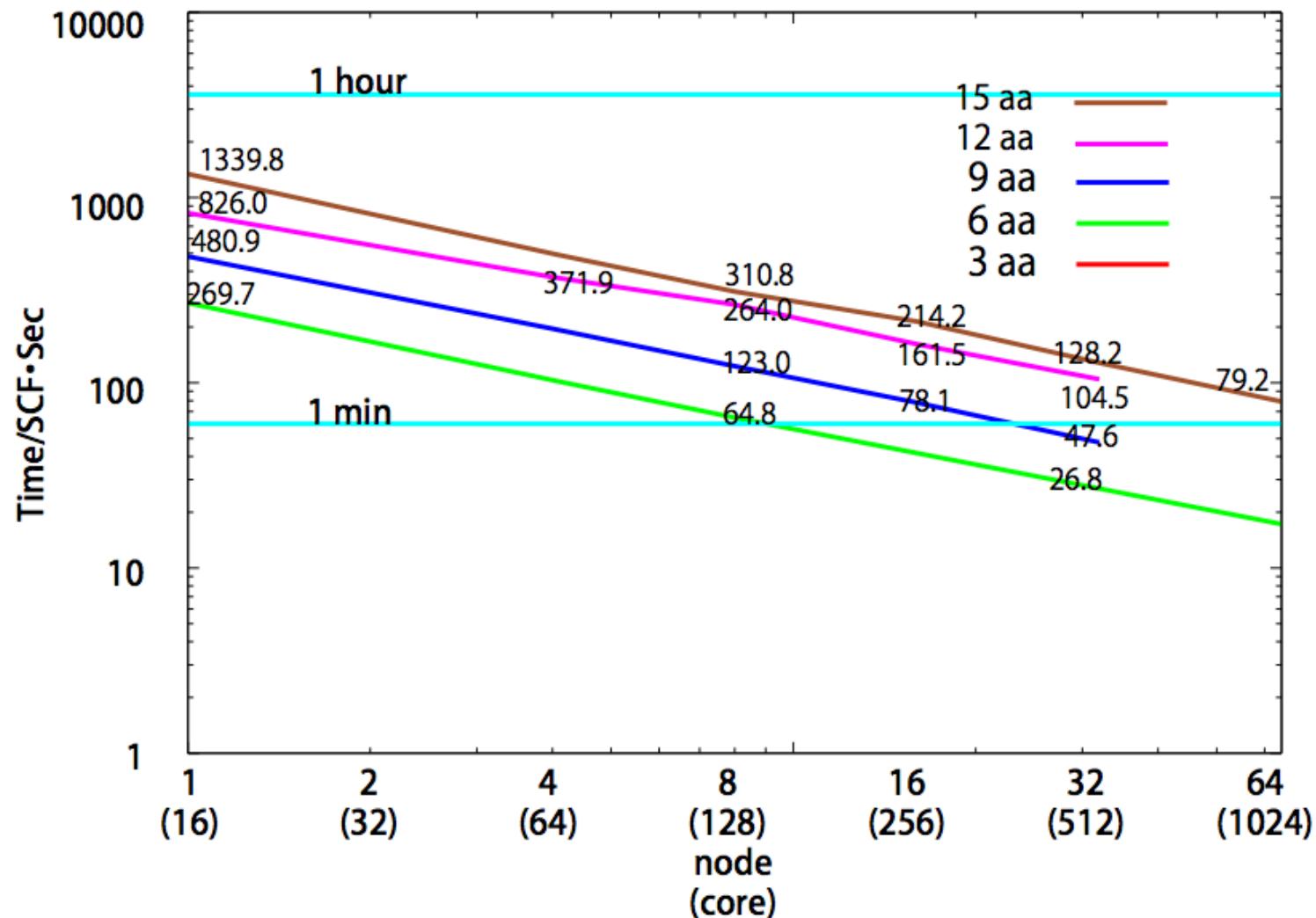
- Opteron (Interlagos)x 2 sockets/node (32core/node) X 2816 node
- 32GB memory/node
- ~800Tflops



T2K-Tokyo (HA8000)



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

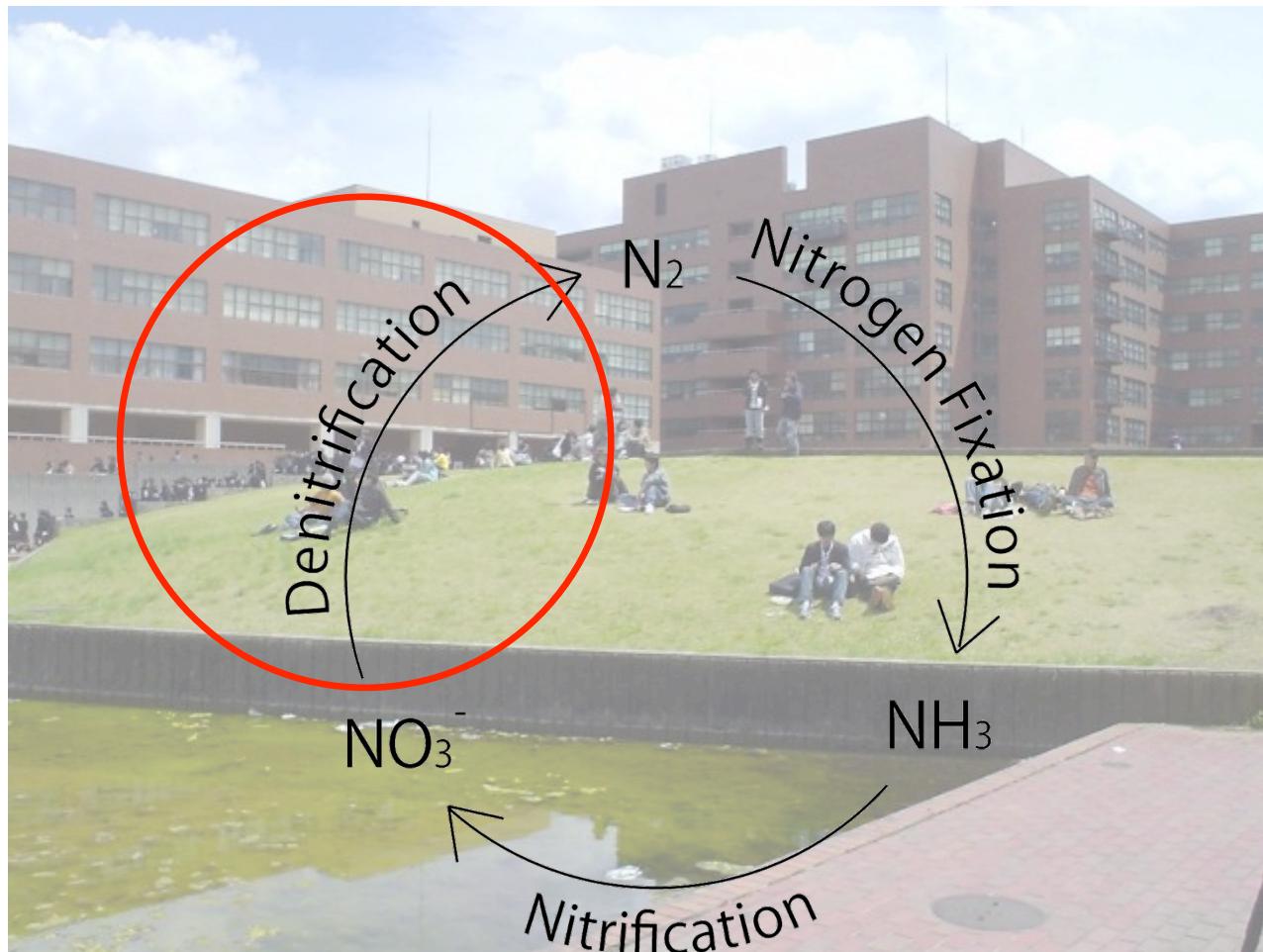


Comparison at a typical case

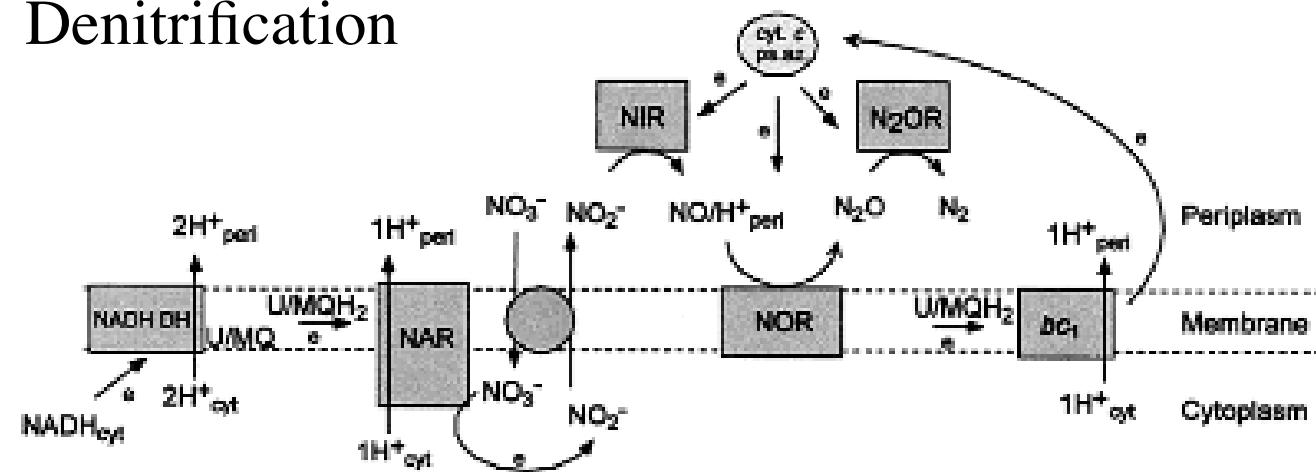
	1SCF/s , 12aa	core(node)
HECToR (Phase3)	87.9	256 (8)
HECToR (Phase2b)	105.8	256 (~10.6)
T2K-Tsukuba	107.2	256 (16)
T2K-Tokyo	161.5	256(16)

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

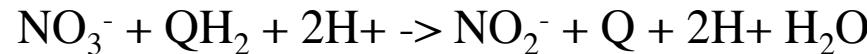
Global Nitrogen Cycle



Denitrification



Nitrate reductase (NAR)



Nitrite Reductase (NIR)



Nitric Oxide Reductase (NOR)



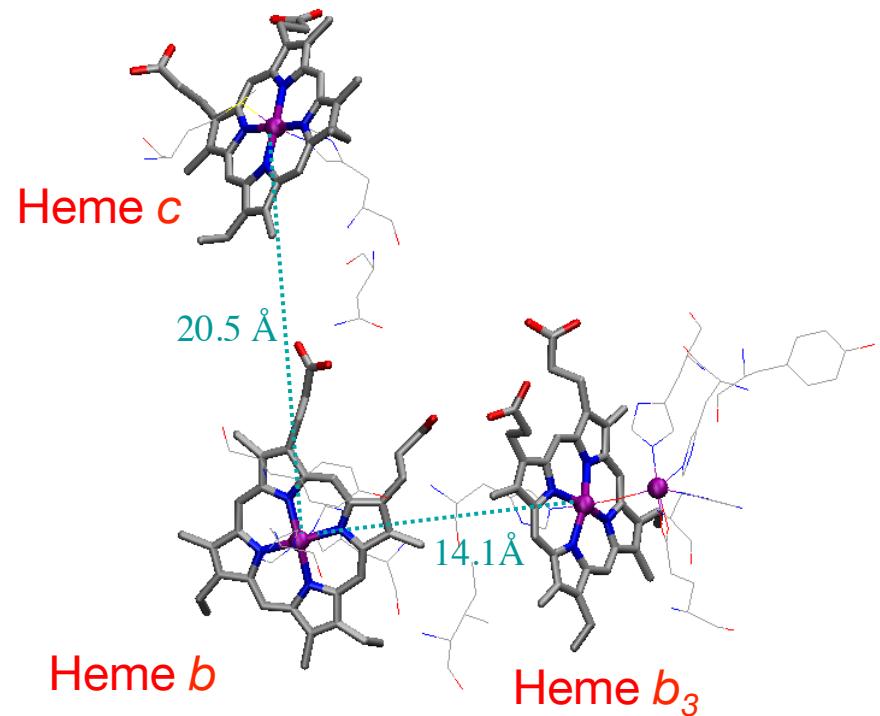
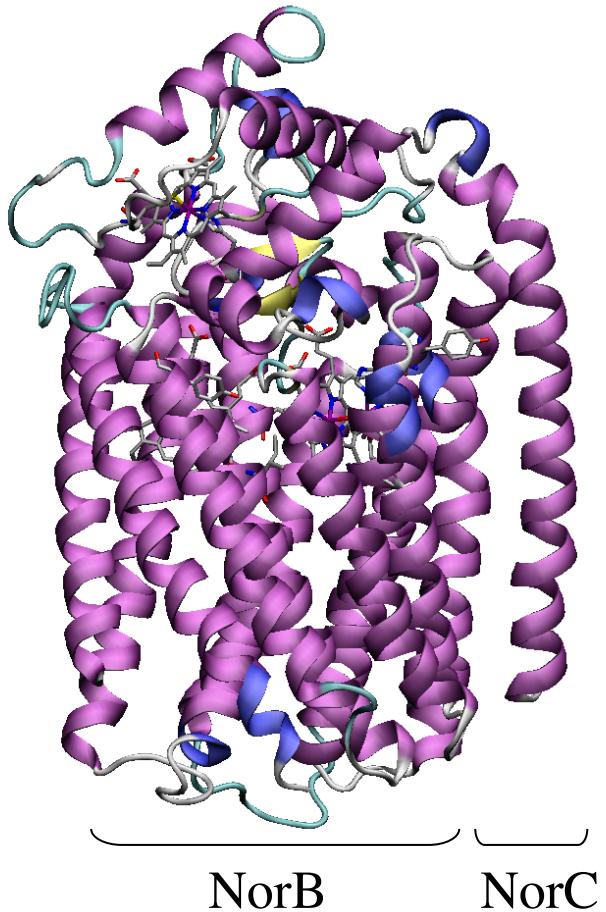
Nitrous Oxide Reductase (N₂OR)



Nitric oxide reductase (NOR)

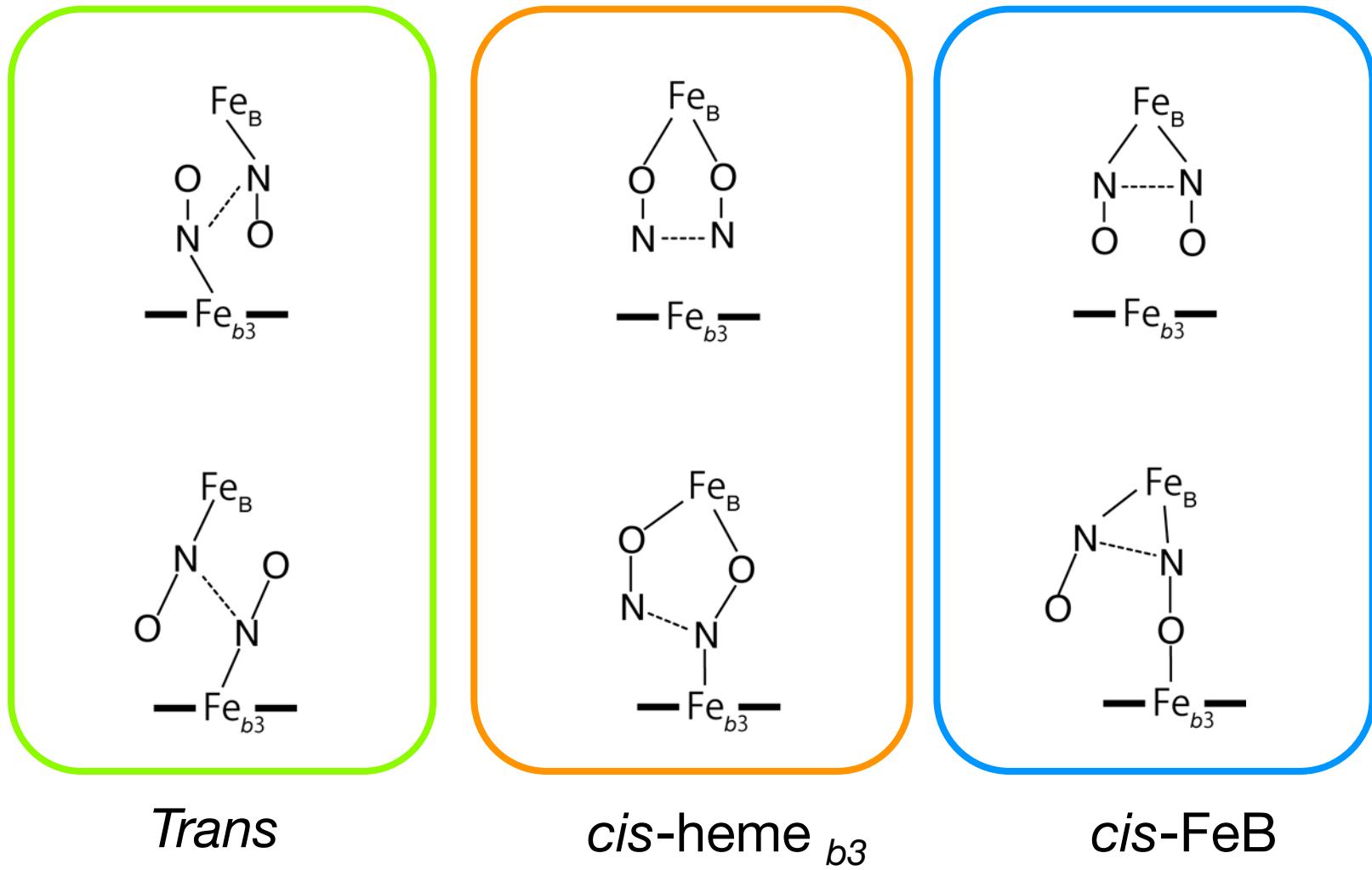
- Reduction of nitric oxide (NO) to nitrous oxide (N₂O)
$$2\text{NO} + 2 \text{e}^- + 2\text{H}^+ \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$$
 - Include a N-O bond cleavage and a N-N bond formation
 - N₂O is a greenhouse gas
-
- First x-ray structure was resolved in 2010 [1].
 - Many similarities 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)

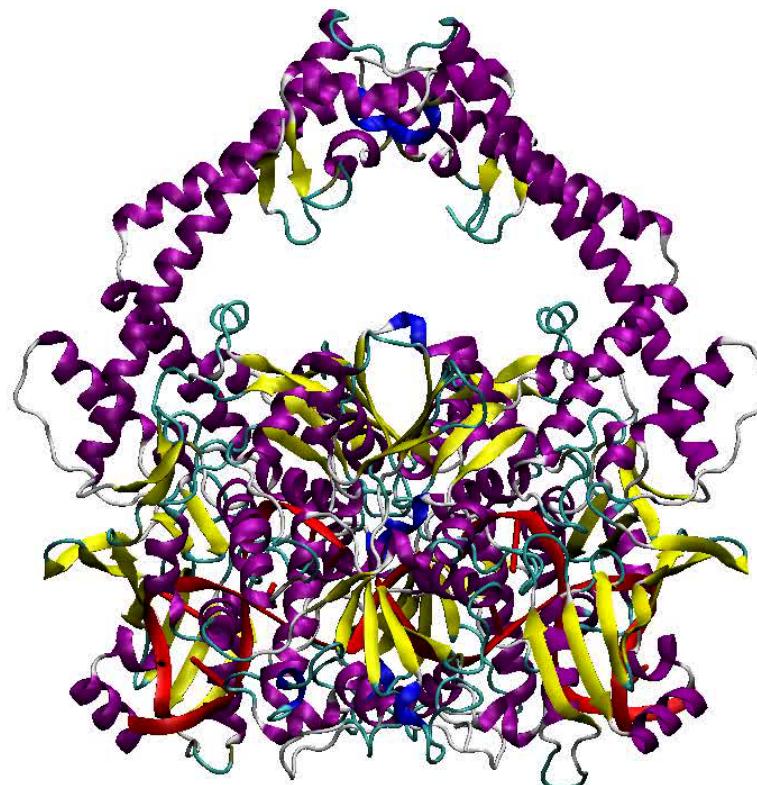
Proposed reaction mechanisms



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

DNA-Topoisomerase

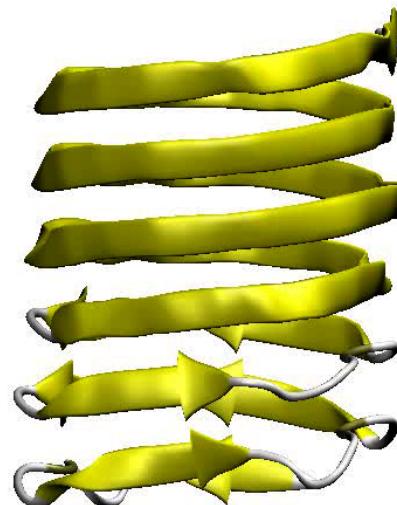
- DNA Topoisomerase: catalyzes interconversions of the different topological forms of DNA
- important drug target for cancer and antibacterial agent



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!