Modeling Biological Hydrogen Production

Breaking the Hydrogen Barrier

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Hydrogen@Home & TFCLS

Presentation Overview

- Hydrogen@Home: **Alpha** Project
  - Conceptual Development
  - Studying Scientific Methods
  - Preparation for Eventual Analysis

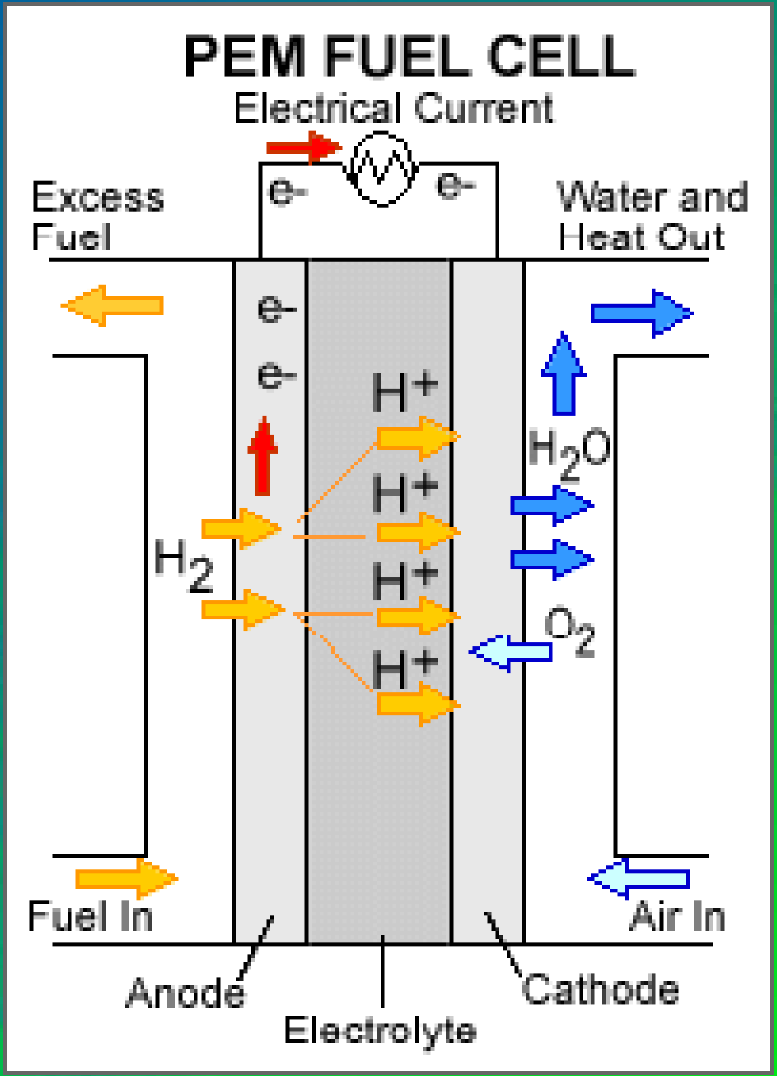
I. Hydrogen: The Energy Carrier
II. Light → Algae → H_2
III. Economy of Scale
IV. Computational Problems
V. Hydrogen@Home Objective

Section I - Hydrogen: The Energy Carrier

- Rationale
  - H2 from water →
    - »Non-Polluting & Renewable = Sustainability
  - Marketability → Technical Hurdles

Hydrogen: The Energy Carrier

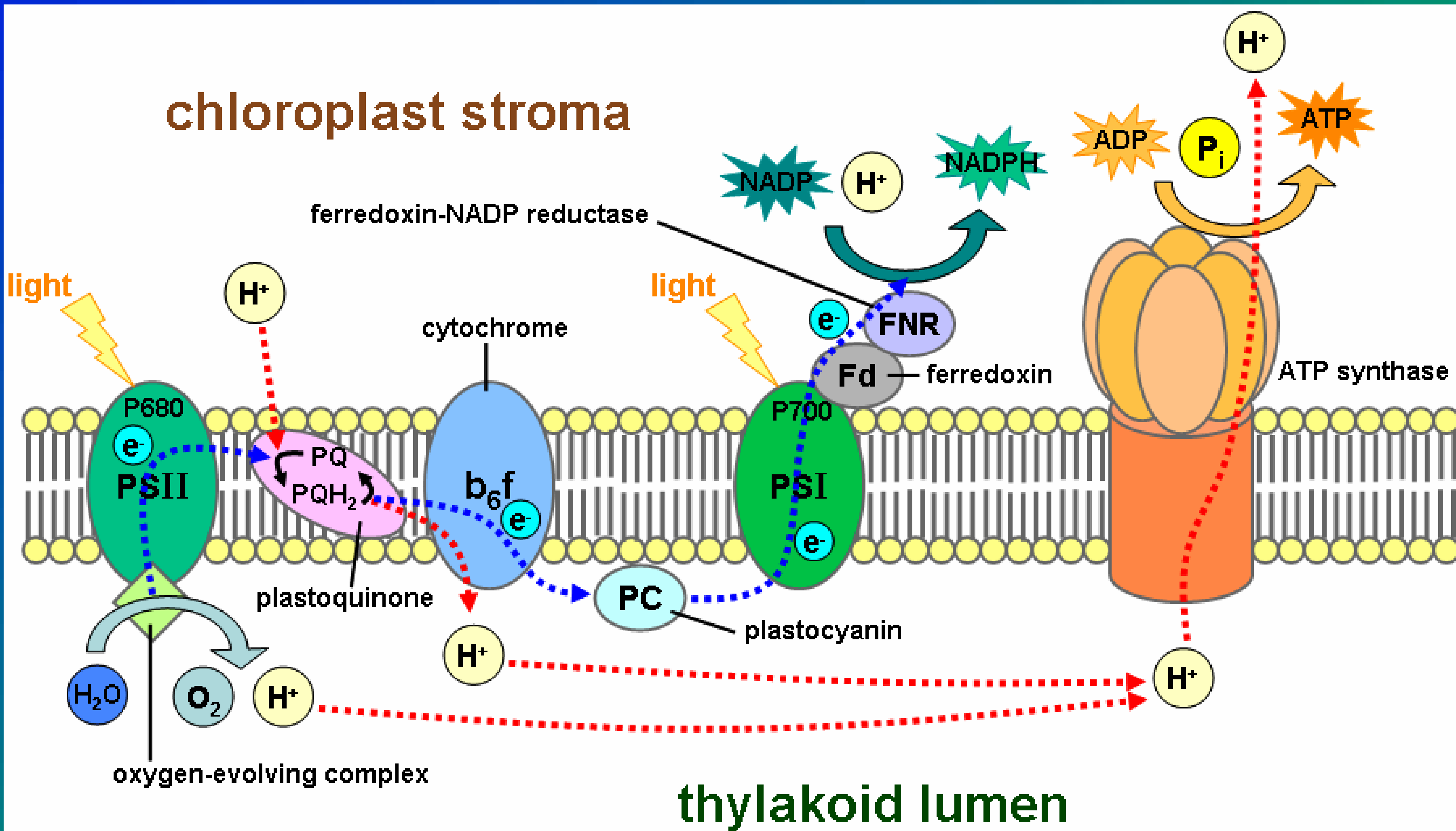
- **Proton Exchange Membrane (PEM) Hydrogen Fuel Cells**
  - **Twice as efficient than Combustion**
  - **Water vapor emissions**
  - **Theoretical 4x as efficient with membrane proteins**



* http://www1.eere.energy.gov

Section II
Light → Algae → H_2
Chlorella Algae Farm

Normal Photosynthesis



Taiz and Zeiger, Plant Physiology, 4th edition

History of Hydrogen

- 16th Century Paracelsus first described H_2
- 1783, Antoine Lavoisier named it Hydrogen
- 1910 - 1914 Hydrogen Zeppelin flights carried 35,000 passengers without incident.
- 1937 Hindenburg destroyed over New Jersey
  - Hydrogen widely assumed the cause
  - Later investigations pointed to aluminized fabric coating & static electricity that ignited.
  - Damage to Hydrogen's Reputation, despite safety measures

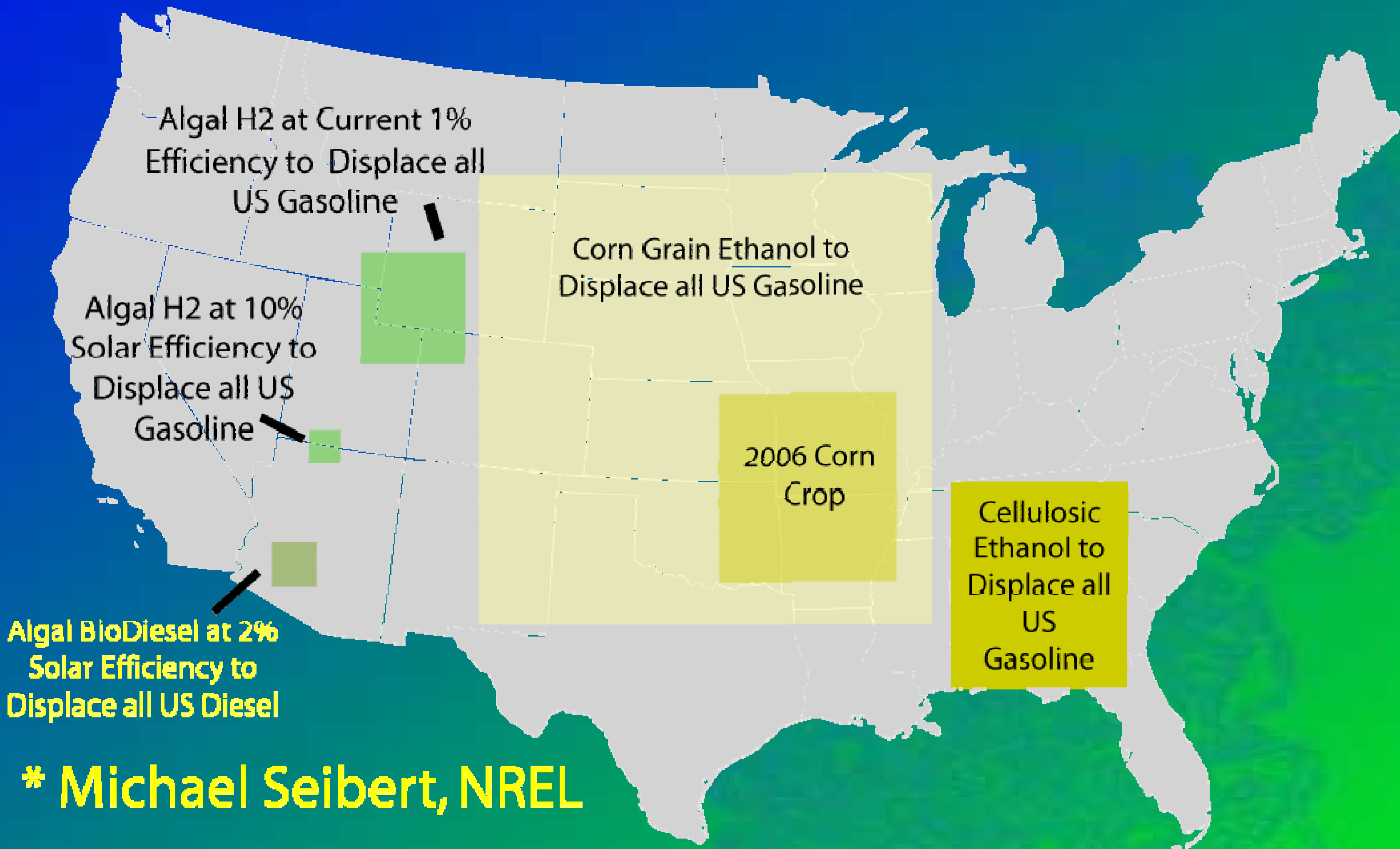
Bio-Hydrogen Milestones

- 1939 Hans Gaffron algae can produce hydrogen.
- 1997 Professor Anastasios Melis deprived sulfur. Hydrogenase, catalyzes reaction.
- 2006 - University of Bielefeld & University of Queensland mutate *Chlamydomonas reinhardtii* produce 5x more. 1.6-2.0 % energy efficiency.
- 2007 - Anastasios Melis achieved 15% Light conversion
- 2007 – Copper added algae produce hydrogen

Some Relevant Research Institutes

Regulation of Genes Required for Nitrogen Fixation in Anabaena Heterocysts	Texas A&M Research Foundation	$ 193,662 NSF 2008
Generating electrical power by coupling aerobic microbial photosynthesis to an electron-harvesting system	University of Maryland Biotechnology Institute	$ 90,000 NSF 2008
Spectroscopic and Computational Mapping of Biological and Biomimetic Hydrogenase Mechanisms	Montana State University	$ 299,691 NSF 2008
Biological Water Splitting, Maria Ghirardi & Michael Seibert	US Department of Energy, National Renewable Energy Labs	

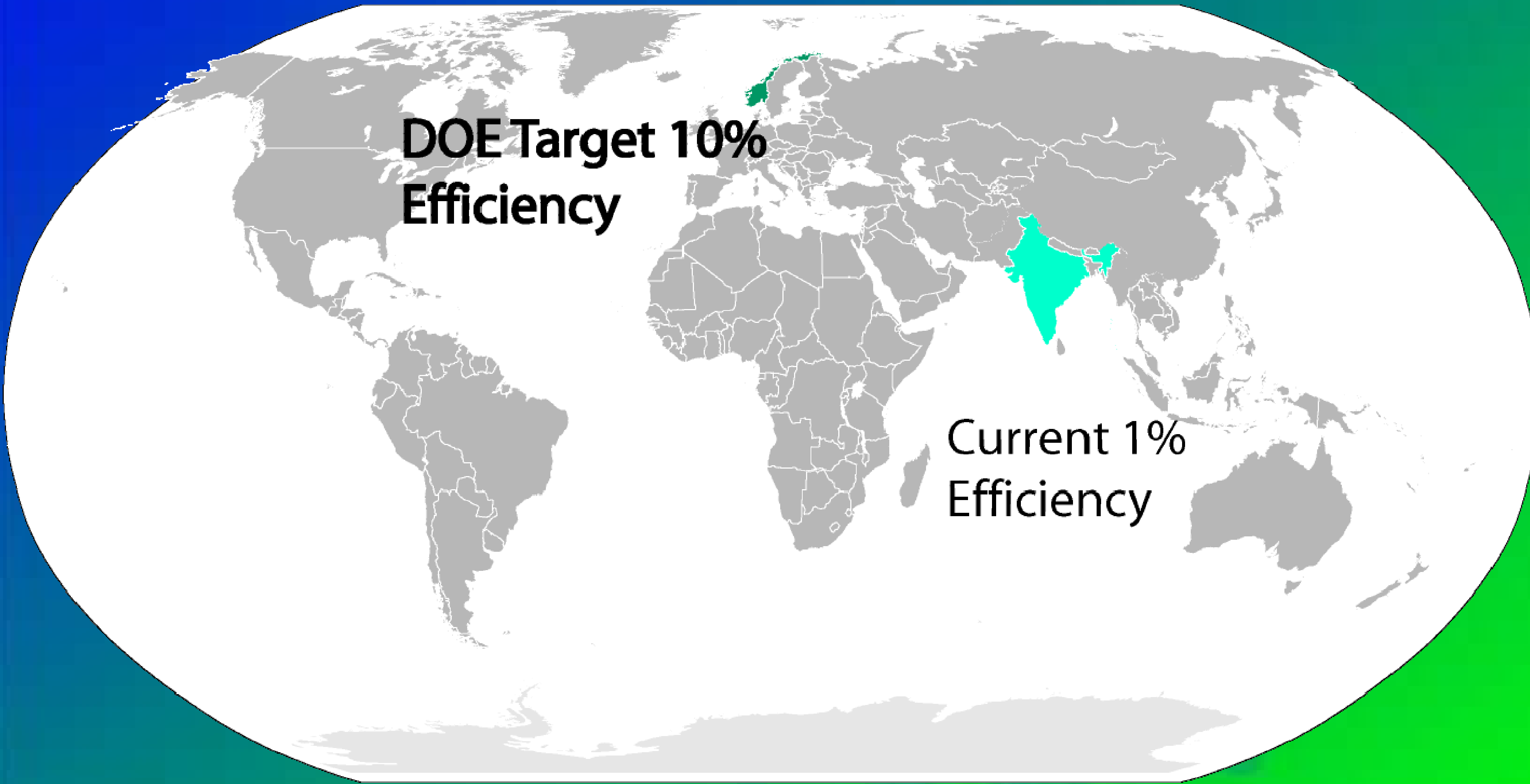
Areas Of Corn Switchgrass and Algal Photobioreactors Required in the US to Displace All Gasoline or Diesel Consumed



* Michael Seibert, NREL

National Renewable Energy Laboratory

Land Requirements for Global Demand



Land Area Requirements

- US DOE Target \$13.53 / kg
- Bio-Reactor Production Rate 2,585 Btu / $m^2 D^{-1}$
- World Primary Energy Consumption (Btu) 2005
  - 462.798 (Quadrillion (10^{15}) Btu) Annual
  - 1.27 (Quadrillion (10^{15}) Btu) Daily Consumption
- Total Land Area Requirements for Daily Consumption
  - 3.46 Million km^2
  - Size of India
- Alternative Approaches
  - Vertical Bio-Reactors
  - Algae grown on Ocean Platforms

http://www.eia.doe.gov/

How to Break the Hydrogen Barrier?

Section IV Computational Problems

- OXYGEN SHUTS IT DOWN!

Purpose of Computer Analysis

1. Improve Understanding of a System
2. Enable Theoretical Predictions

Relevant Applications for NREL

- Computational Material Science (VASP, Wien2k)
- Computational Chemistry (Gaussian, NW Chem)
- Computational Biology (Charmm)
- Large Scale Molecular Dynamics (NAMD)
- Computational Fluid Dynamics (Ansys, Fluent)
- Scientific Libraries (LAPACK, BLAS, FFTs, HDF (Hierarchical Data Format))
- Docking Simulations (FTDock, AutoDock)

Applications For Hydrogen@Home

- Sequence Analysis – BLAST
- Protein Structural Homology Analysis
- Model Molecular Affinities – Docking
- Probabilistic Molecular Behavior – Monte Carlo
- Deterministic Molecular Behavior – Molecular Dynamics (Semiempirical QM & MM)

Topics to Study

1. Enzyme Screening & Enzyme Design
   - Need Better Understanding of Reaction
   - Difficult to Automate Analysis
2. Oxygen Diffusion Studies
   - Many approaches
   - Published methods Molecular Dynamics
   - Possibility to Compare Simulations w/ Empirical evidence

Oxidation Mitigation Approach (OMA)

- Oxygen membranes transport
  - Analogous to Competitive Inhibition of Enzymes except reversed
  - Docking Oxygen to Protein competing for Oxygen against Hydrogenase
  - Molecular Dynamics of Protein Oxygen Complex

Resource Requirements

- OMA requirements for Docking & Dynamics
  - Protein Data Bank > 50,000 & growing
  - Narrow to membrane proteins < 3,000
  - ~100 different Docking parameters each interaction
    - 1 hr simulation time
  - ~100 MD Each Docking complex
    - 8 hrs to simulate 250 ps, w/ 50,000 atoms, 2 CPU
  - Nano-timescale for all simulations – Brute Force
    - 200,000 CPU years plus error checking
    - We must filter our data sets

Unknowns & Project Requirements

- Resources Requirements for Force Field Parameterization
- Method for Automating our Molecular Dynamics analysis
  - Formatting Protein Files, < 10,000 atoms
  - Guessing appropriate simulation parameters
- Quality of Predictions
  - Need benchmark laboratory comparisons
  - How to measure statistical relevance

Success Stories

- Integrating Autodock4
  - User interface for Docking Simulations
  - Analyzed Ferredoxin Binding to Hydrogenase
- Integrating CP2K for Molecular Dynamics
  - Ran Test workunits
  - Looking to improve integration
  - Studying ways to automate MD

Section V
Hydrogen@Home Objectives

- **PASTA** – Past, Present & Future
  - Production
    - Enzyme models – Too Problematic for now
    - Screen for O_2 transport – Exploring
  - Application - Eventually model proton transport enzymes
  - Storage &Transport - looking for ideas
  - Assess Environmental Impact
    - Will Model H_2 Behavior in Ozone
    - Will Model Impact caused by Algae

For Extra Fun

- http://www.youtube.com/watch?v=r9vniN54Aok

Thank You

- David Anderson, Carlos Barrios-Hernández, Derrick Kondo, Arnaud Legrand
- Special Thanks to NREL researchers Maria Ghirardi & Mike Seibert