

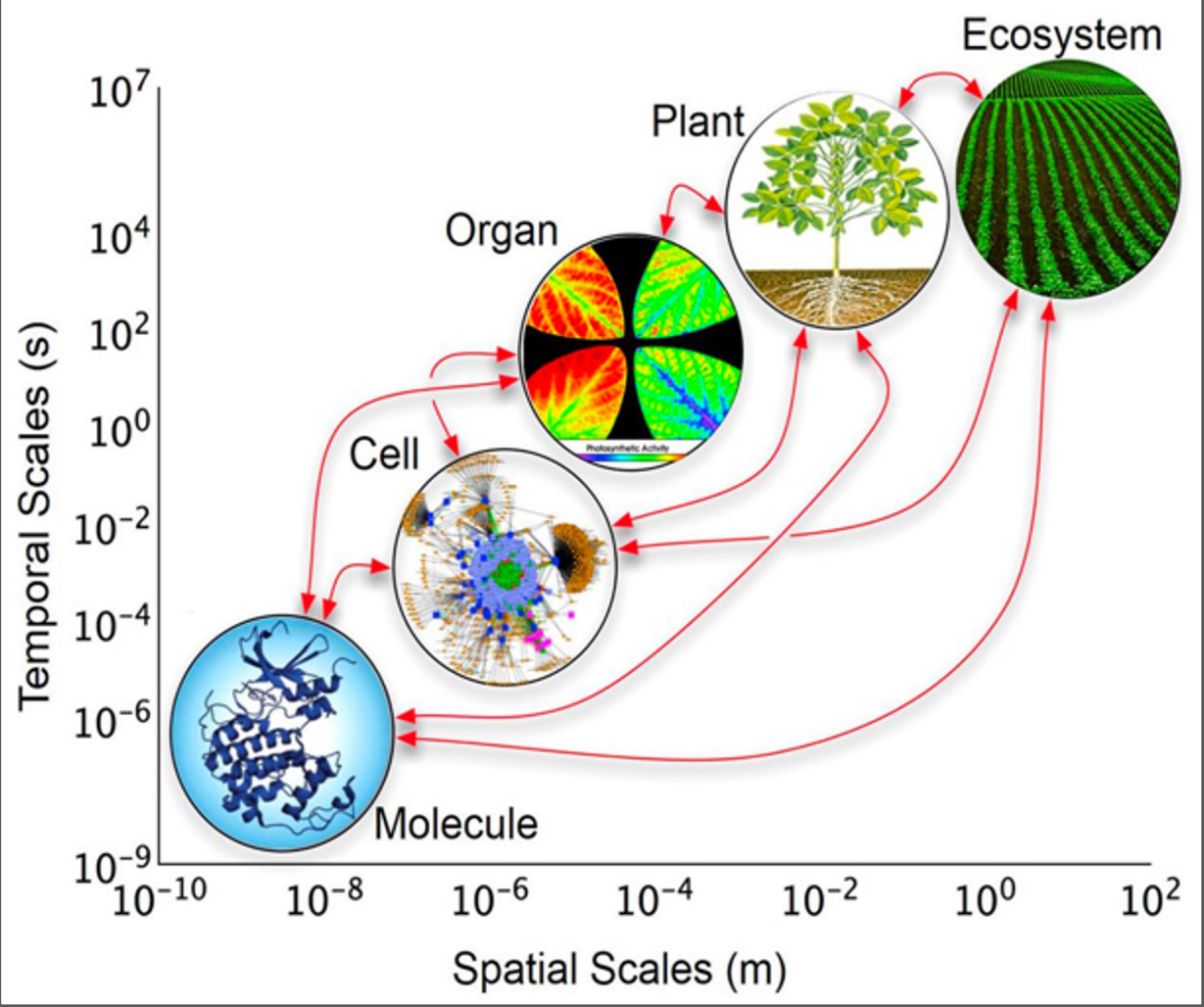
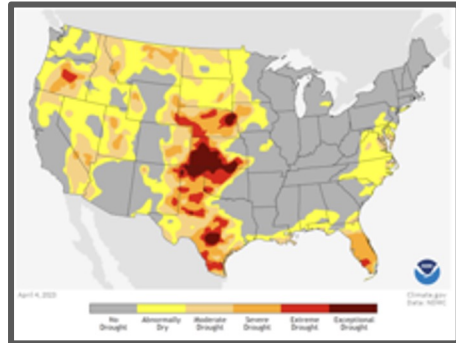
Characterizing Variation of PSII Water Channels Between Cyanobacteria and Higher Plants

Benjamin Romanjenko, Jose Ortiz Soto,
Carmela Guadagno, Marilyn Gunner

ERPC, April 15, 2023



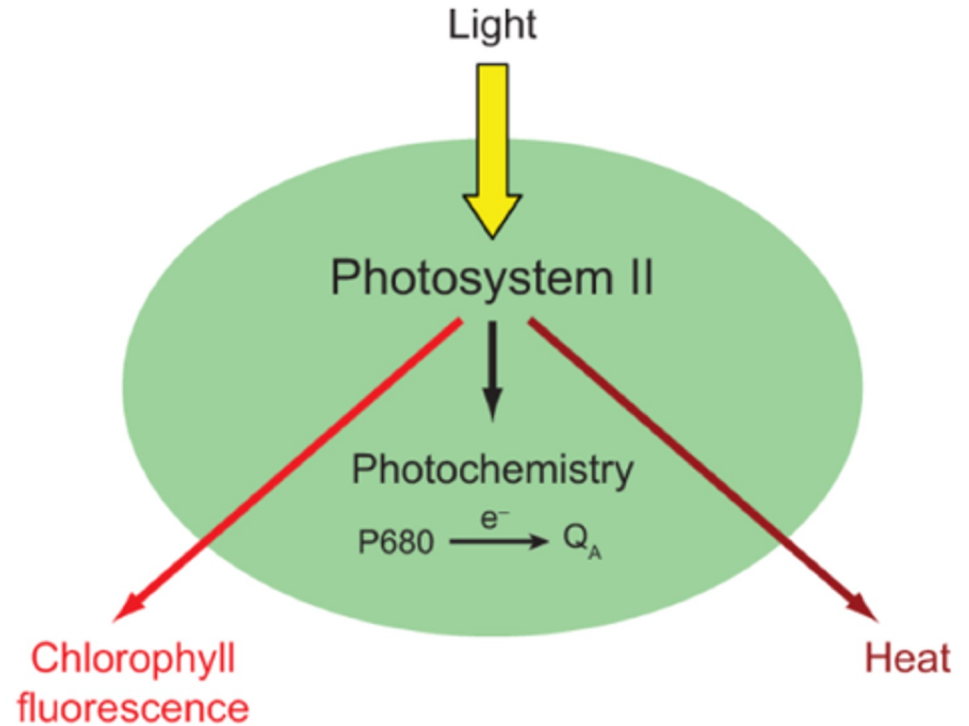
The Big Picture



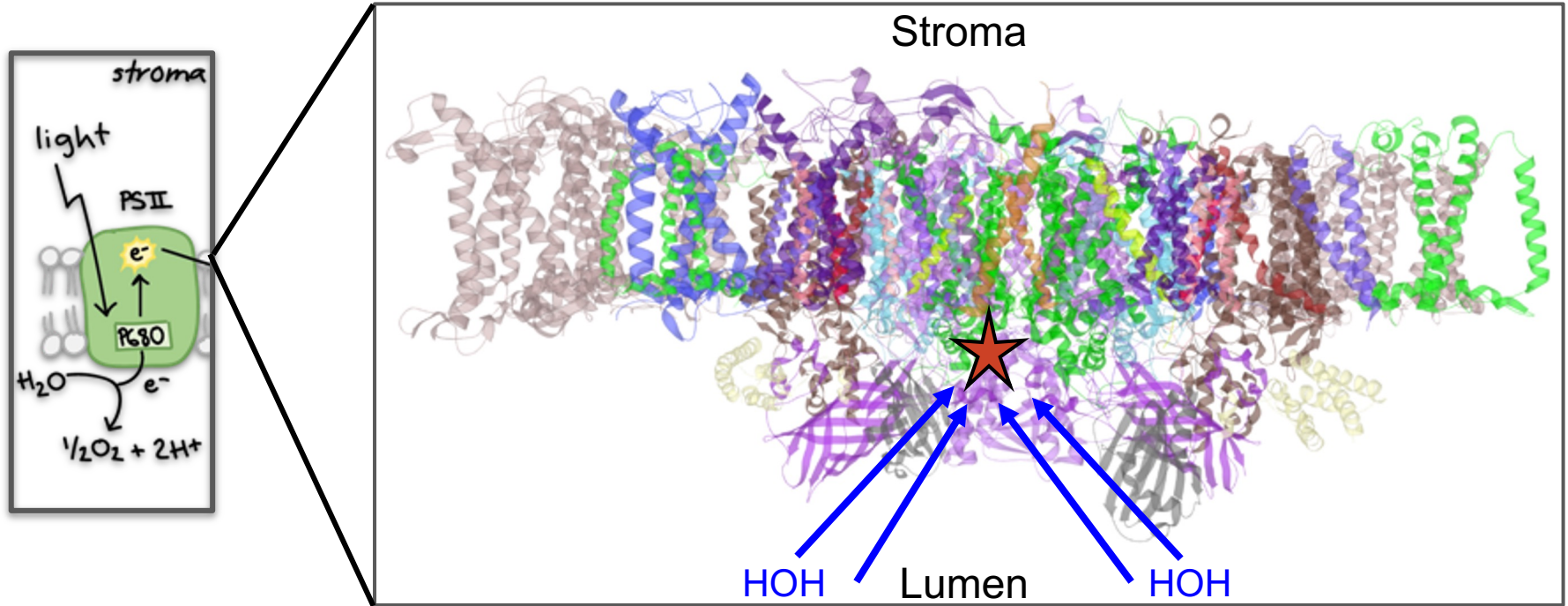
Chl a Fluorescence

Light Energy (3 Options)

- Photosynthesis
- Heat
- Fluorescence



Water Channels



What has been done with Water Channels

Publication	Structure	Method
Sirohiwal and Pantazis 2022	3WU2, 3I4D, 5B66, 5TIS	MD
Kaur et al., 2021	4UB6	MCCE
Hussein et al., 2021	7RF1, 3JCU, 4UB6, 6JLJ	RT crystallography, Caver 3.0
Cardona et al., 2015	Cyano	Phylogenetics
Vassiliev et al., 2013	3ARC	MD

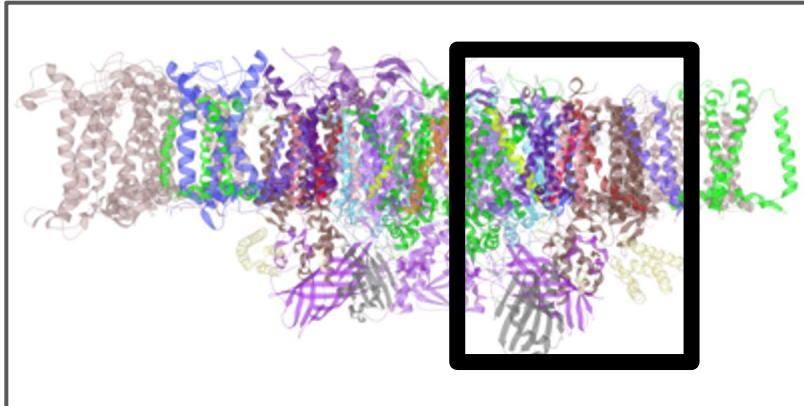
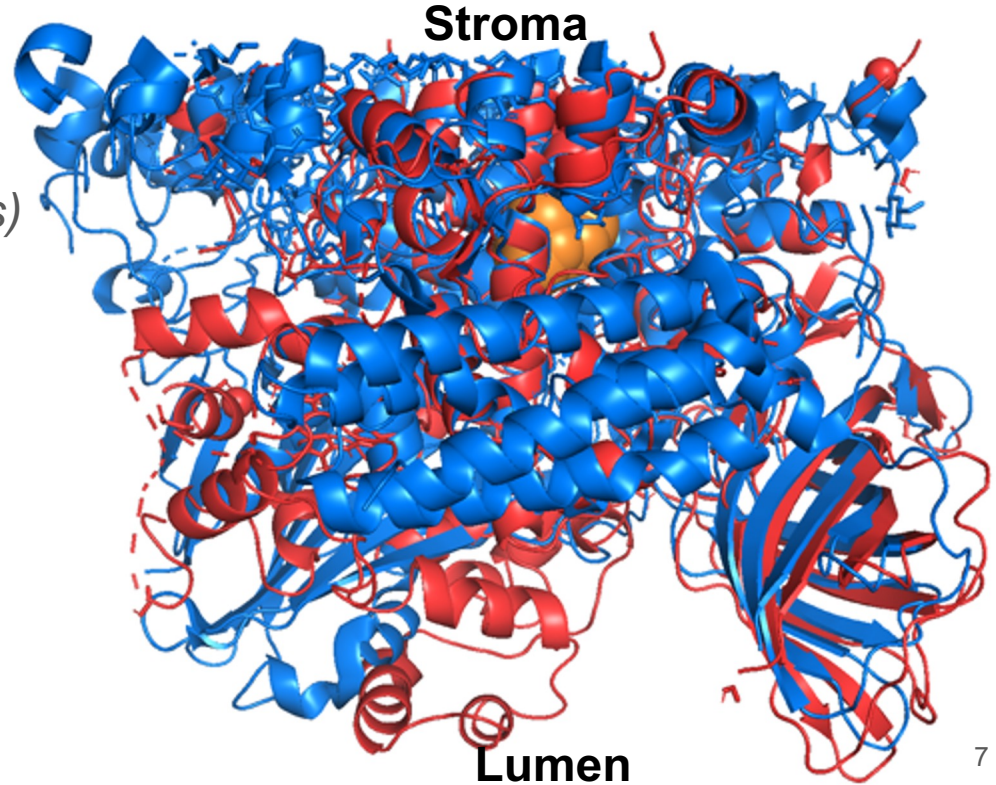
Higher Plants: 3JCU

Q: Is there variation in water channels?



PSII Differences

- Oxygen Evolving Complex: Orange
 - 5XNL (*Pisum sativum*)
 - Blue
 - 4UB6 (*Thermotichus vulcanus*)
 - Red



T. vulcanus

Stroma

Pea

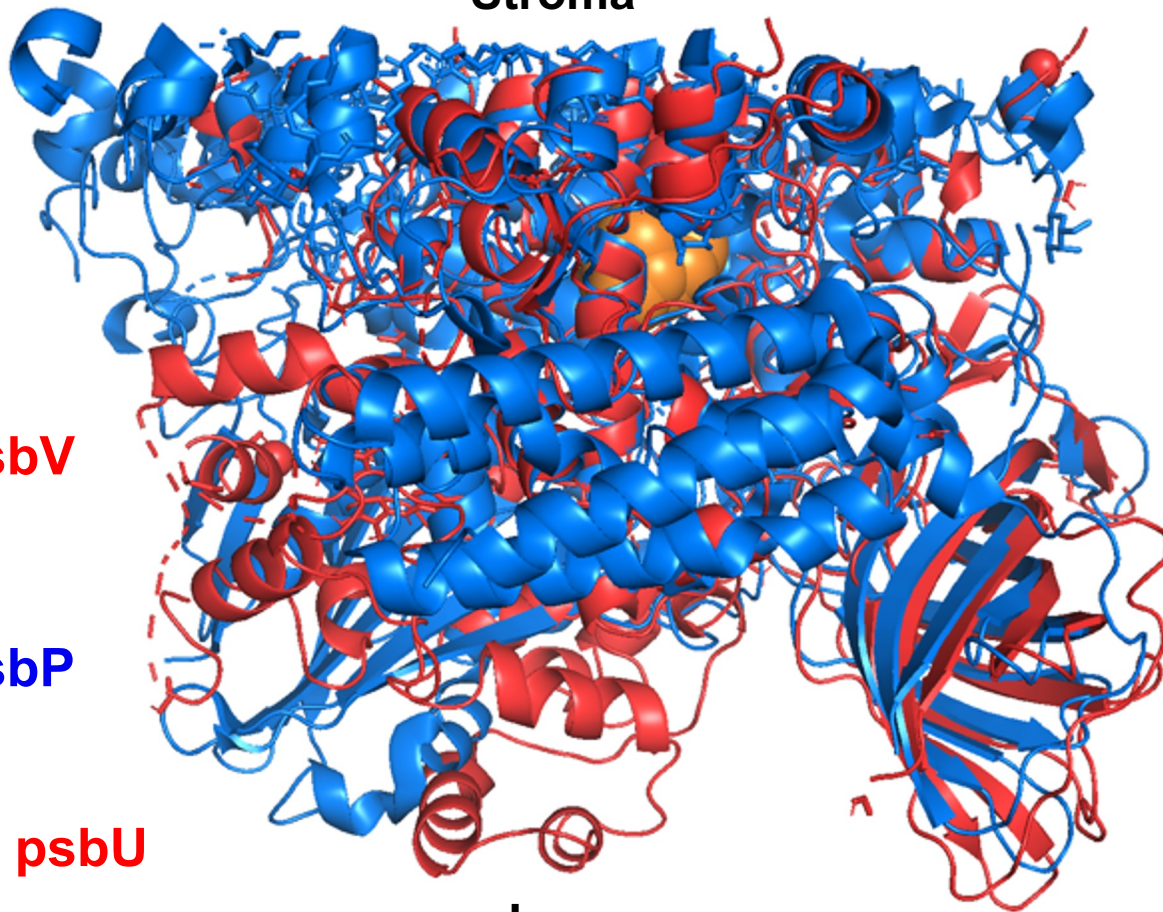
psbV

psbP

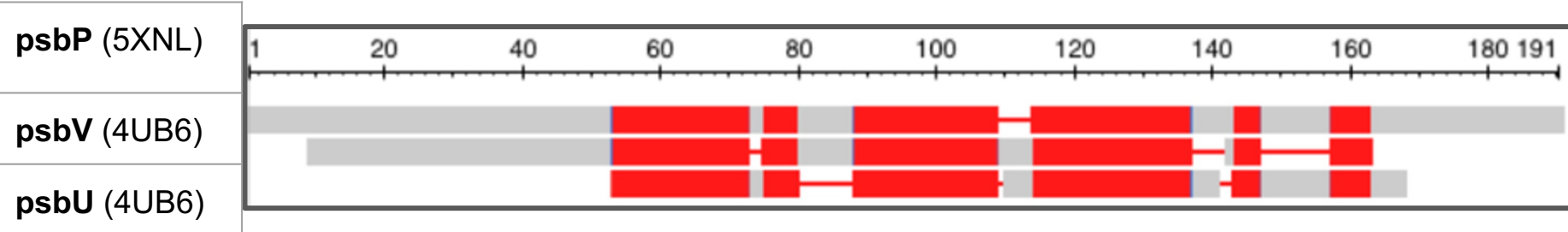
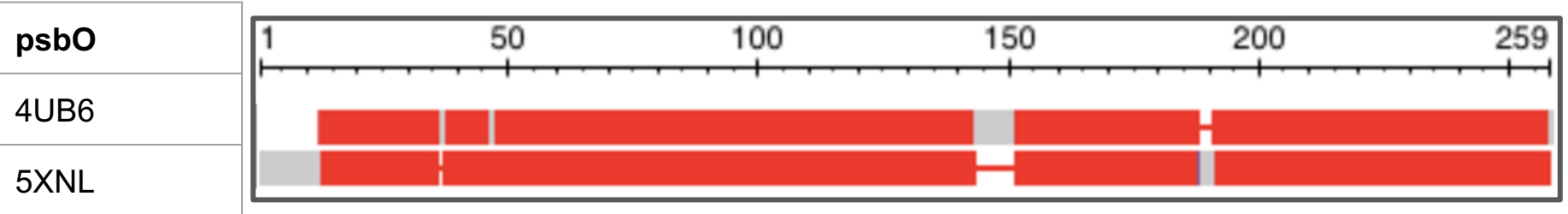
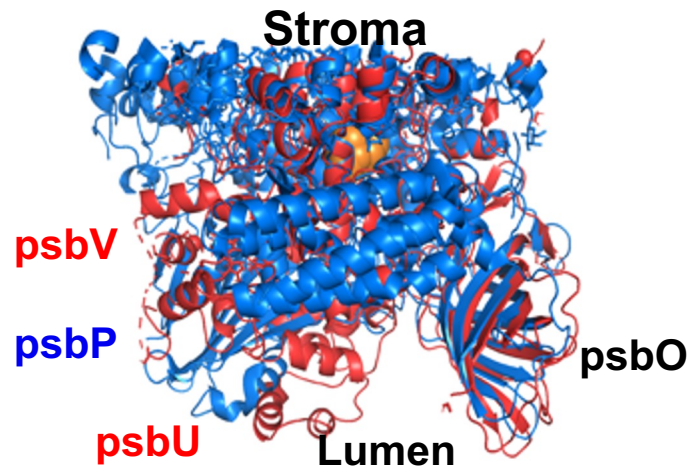
psbU

Lumen

psbO

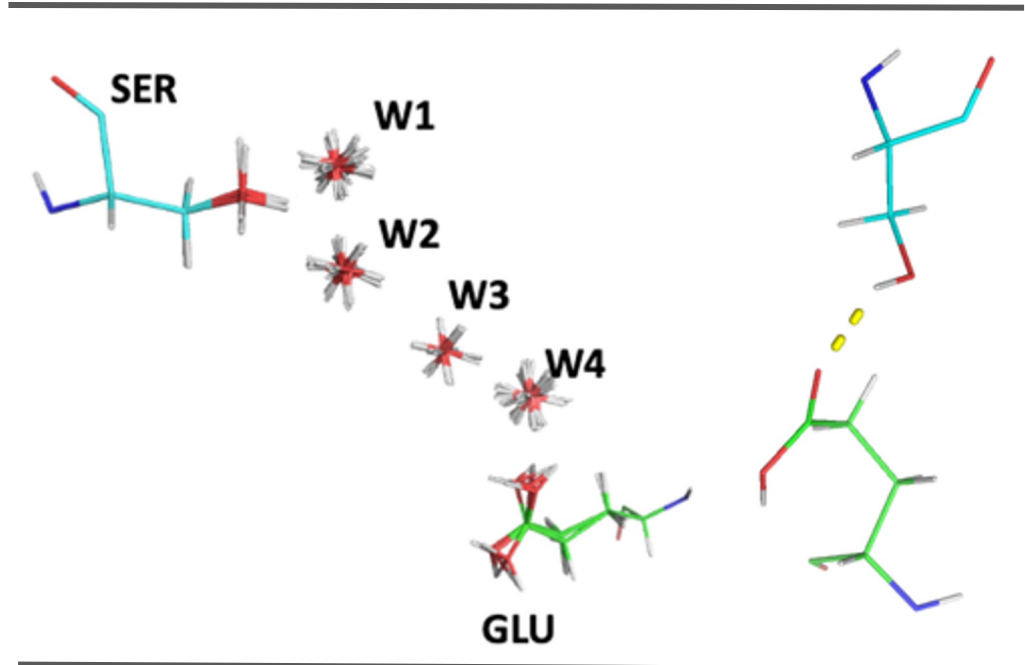


PSII Differences



Multi-Conformational Continuum Electrostatics (MCCE)

- Sample multiple protonation and conformation states
 - Side chains
 - Waters.
- Determines probability of conformations and make hydrogen bonds
- Hydrogen bonds are organized into networks

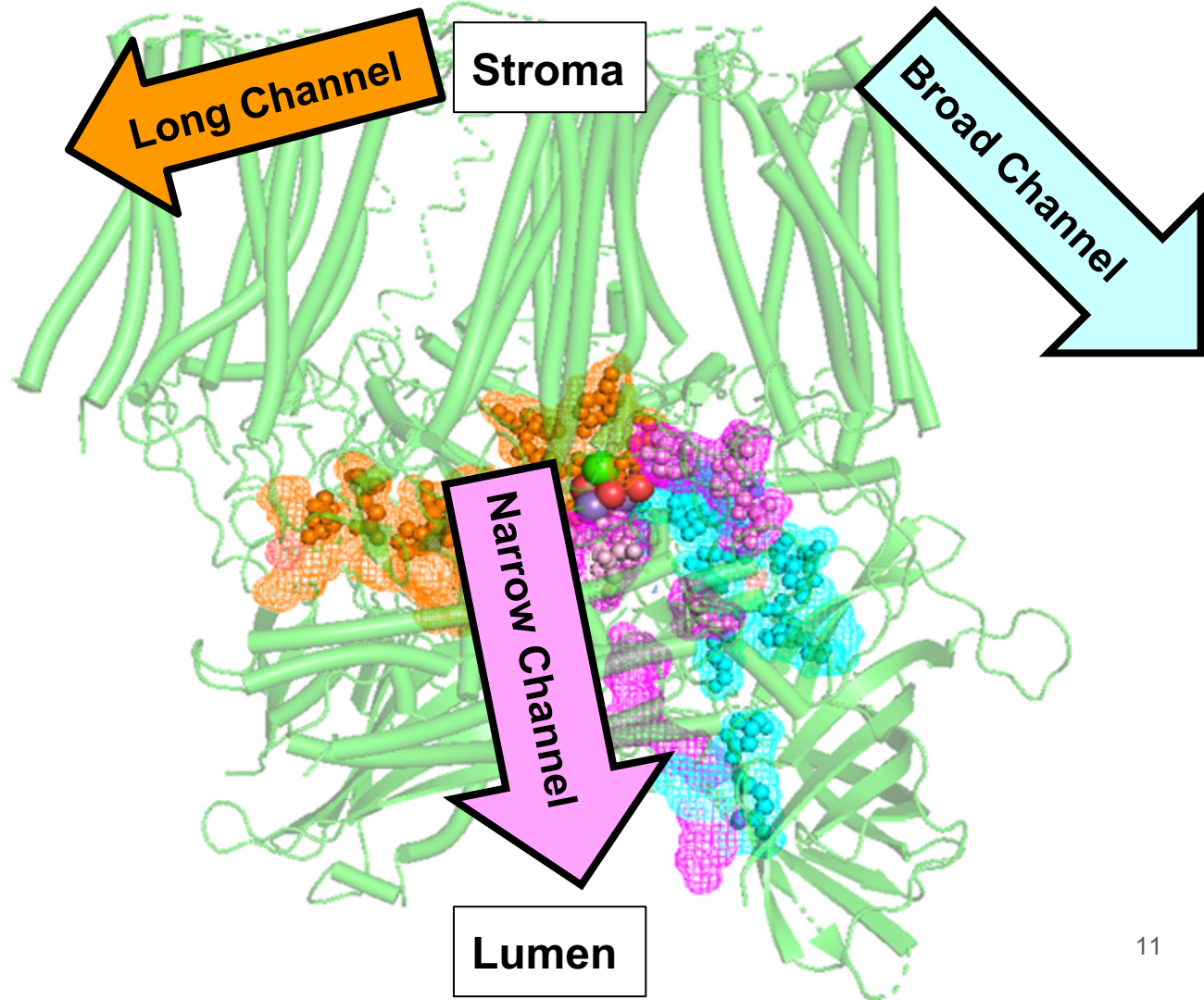


Gunner Lab, Kaur et al., 2021

Current Network

Mesh = *T. vulcanus*

Spheres = Pea 'match'



Amino Acid Variation

4UB6(<i>T. Vulcanus</i>) ⇨ 5XNL(<i>Pea</i>)		
Large	Broad	Narrow
SERP39 ⇨ THRC397	ASPM102 ⇨ ASPO110	SERA85 ⇨ THRA85
LYSP47 ⇨ LYSP170	ASPM99 ⇨ ASPO107	GLUO93**
LYSO104 ⇨ GLYO164	GLUM97 ⇨ GLUO105	ASPO96**
LYSP103 ⇨ PROQ32	GLUD312 ⇨ GLUD313	
	GLUD310 ⇨ GLUD311	
	ASPD222 ⇨ ASPD225	
	HISM228 ⇨ ASP227	
	ASPD308 ⇨ ASPD309	
	ASPD224 ⇨ ASPD227	
	LYSM188 ⇨ LYSO191	

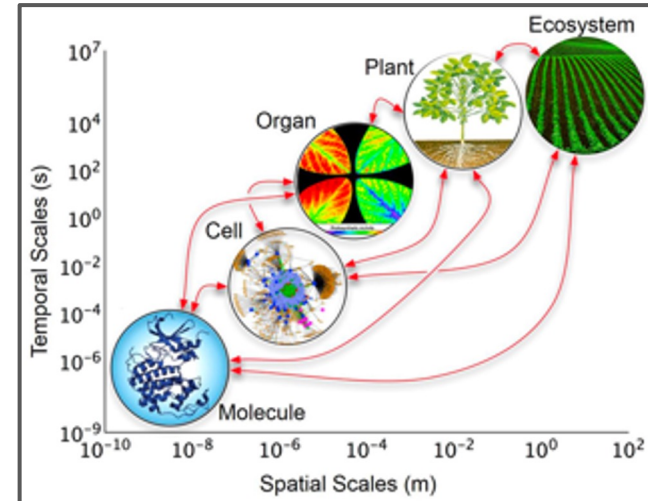
Future Direction

- Re-run MCCE
 - With crystal waters
 - With saturating waters



If there are difference

- Repeat with other higher plant PSII structures
 - Characterize channel variation



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- NIFA AG2PI Collaborative (2021-704-35233)
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- University of Wyoming, School of Graduate Education
 - Travel Funding

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Collaborators: Jose Ortiz Soto, Marilyn Gunner





NSF RESEARCH-PGR
#2102120

Questions

