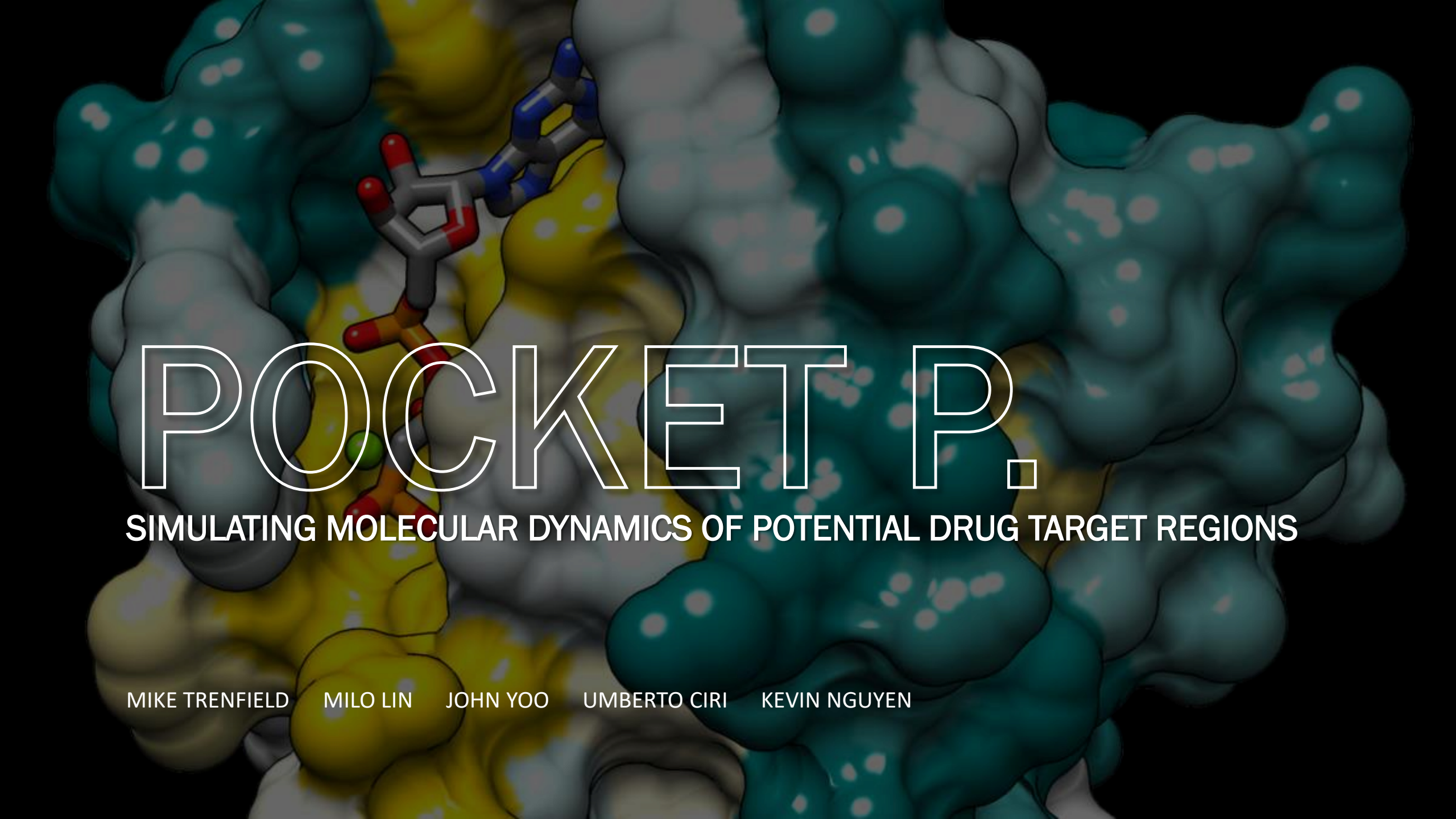


POCKET P.

SIMULATING MOLECULAR DYNAMICS OF POTENTIAL DRUG TARGET REGIONS

MIKE TRENFIELD MILO LIN JOHN YOO UMBERTO CIRI KEVIN NGUYEN

DEFINING THE PROBLEM

RAS FAMILY OF G-PROTEINS

- UNDRUGGABLE
- LACK OF BINDING POCKETS
- UNEXPLORED DYNAMIC STRUCTURE

GOAL

IDENTIFY THE SHAPE & LOCATION OF TRANSIENT POCKETS

SCOPE

DATA ANALYSIS

LOCATE POCKET

FIND VOLUME OF POCKET

TRACK POCKET STABILITY OVER TIME

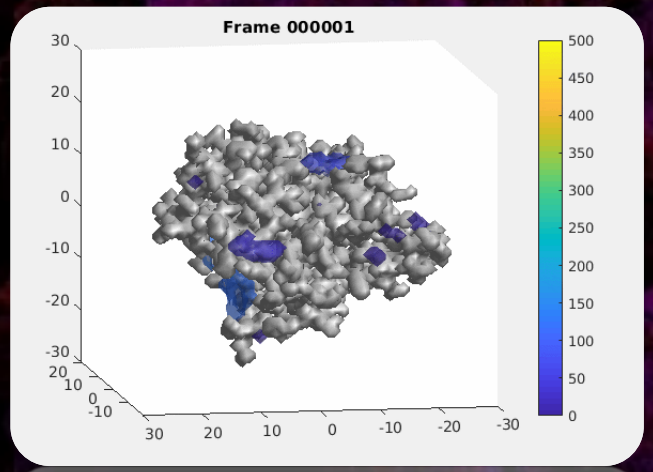
VISUALIZATION

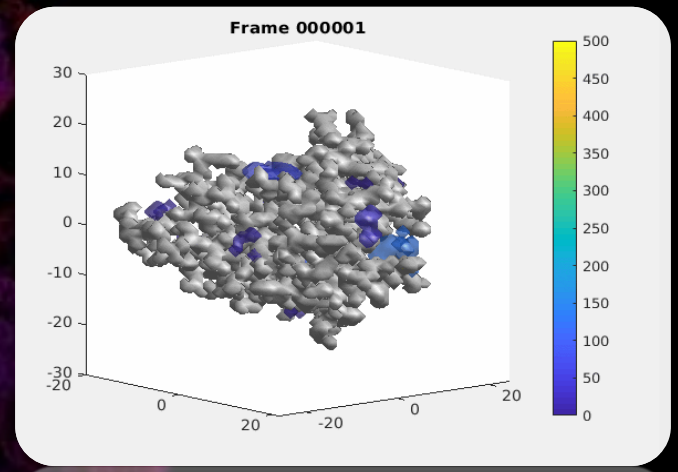
3D IMAGE OF EACH FRAME

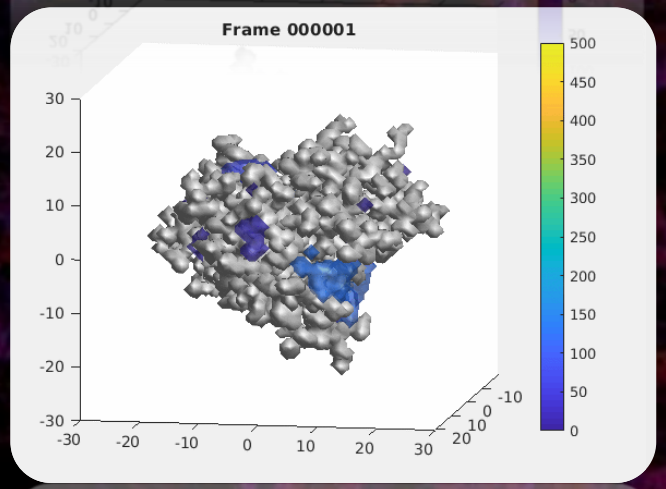
REAL TIME VIDEO MODUEL

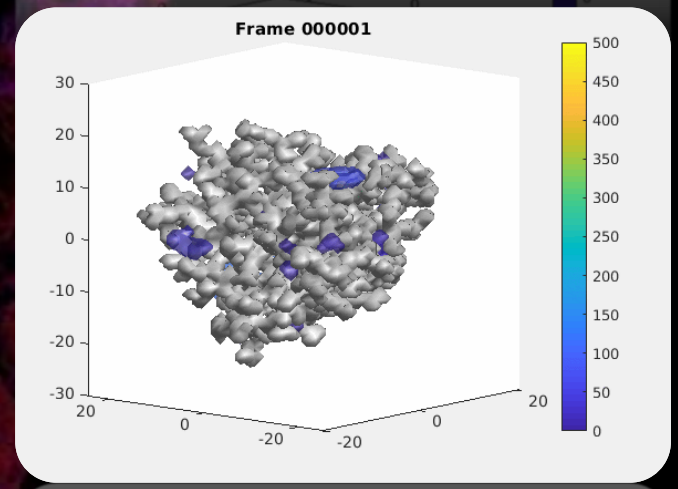
VISUALIZATION

20 microsecond long simulation



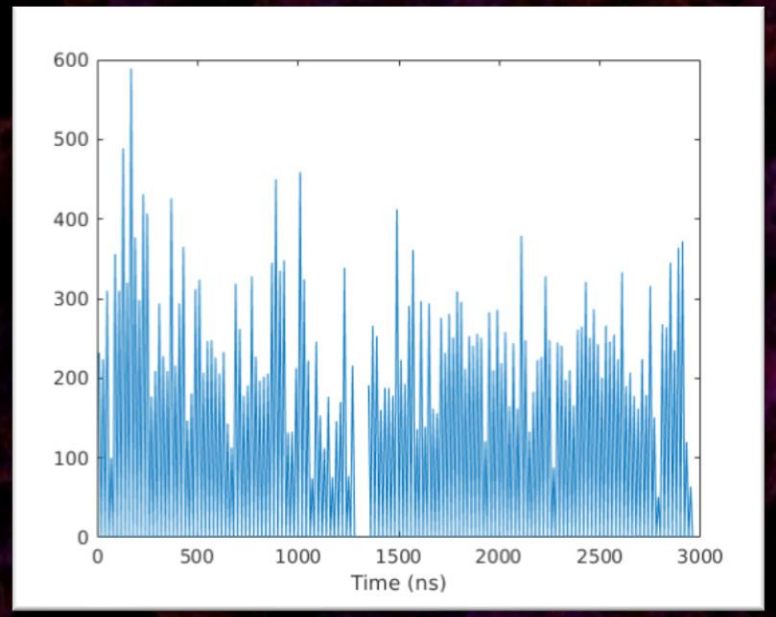






DATA ANALYSIS

EXAMPLE OF DISCOVERED POCKET



POCKET VOLUME OVER TIME

PYMOL RENDERING OF POCKET