

What Do You Do When Two Hands Are Not Enough?

Interactive Selection of Bonds between Pairs of Tangible Molecules

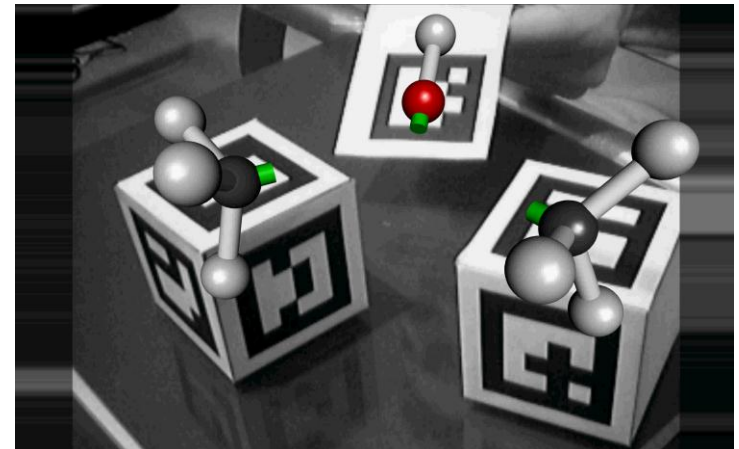
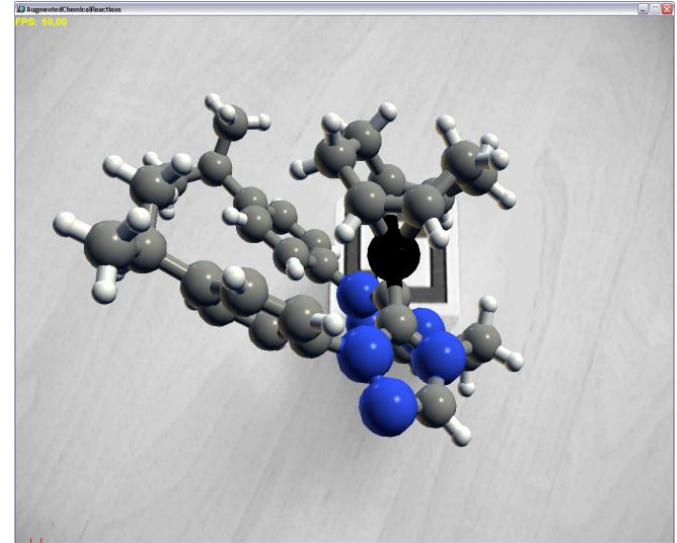
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Overview

1. Project “Tangible Chemical Reactions”
2. Problems with Two Handed Interactions
3. Problem in Selecting with Controlled Objects
 - Proximity Based Selection
 - Shake Based Selection
4. Evaluation and User Study

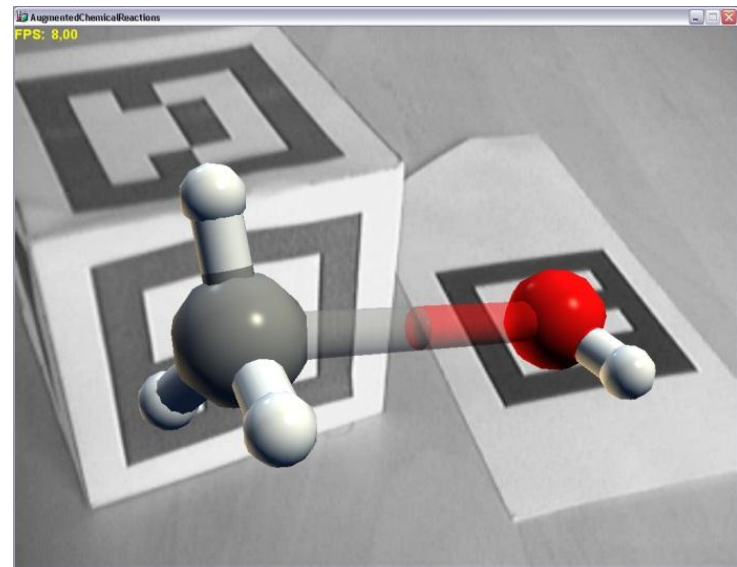
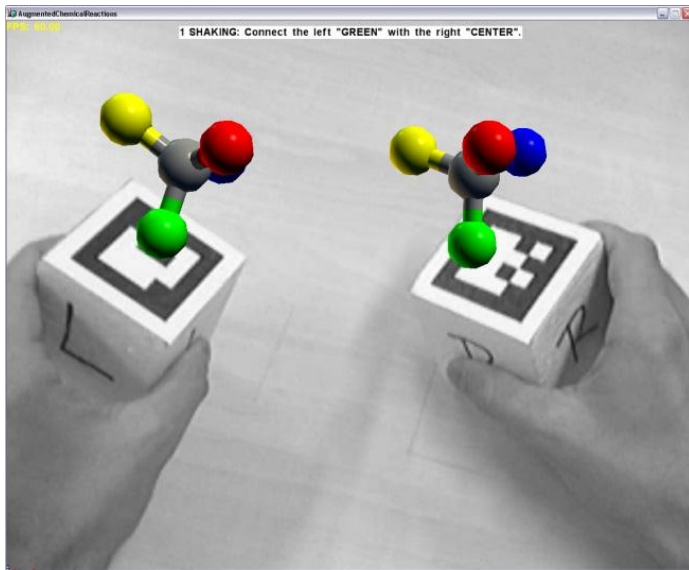
Project “Tangible Chemical Reactions”

- Intention:
 - Help chemists in designing catalysts
 - Help students in learning/understanding chemistry
- Methods:
 - Visualize and control models of molecules in 3D
 - Show the dynamic behavior of the molecules
- Desired results:
 - Speed up the process of designing new molecules
 - Help to improve the understanding of chemistry

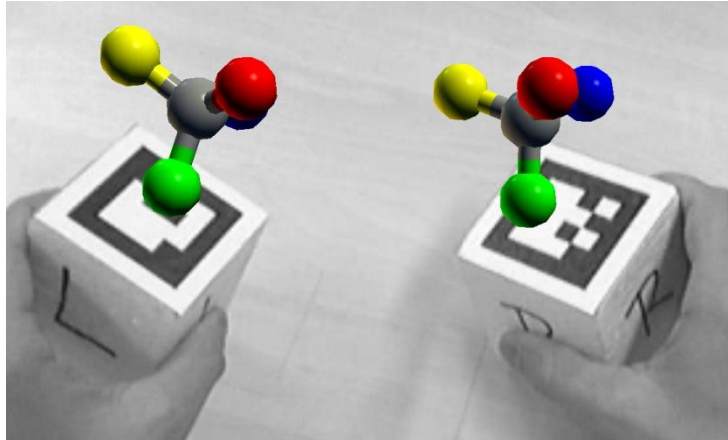


Project “Tangible Chemical Reactions”

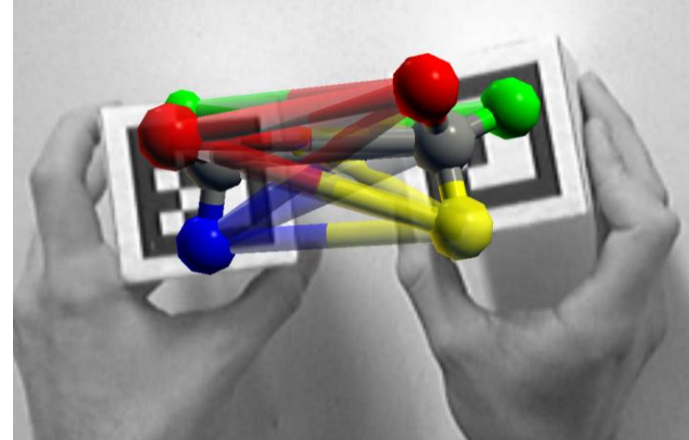
- Show molecules on top of the markers.
- Possible bonds are shown (right picture)



Problem in Selecting a single Bond between Molecules



Separate molecule models



All possible bonds are shown

Problem:

- How to select one possible bond out of the whole set of possible bonds?

Problems with Two Handed Interaction

- Only two hands available
- Hands occupied by holding the markers
- How to tell the system to select or trigger an event on a controlled object?

This could be done in several ways: Speech, foot pedals, putting on table, ...

But we focus on gestures, when hands are not free.

Selection with Controlled Objects

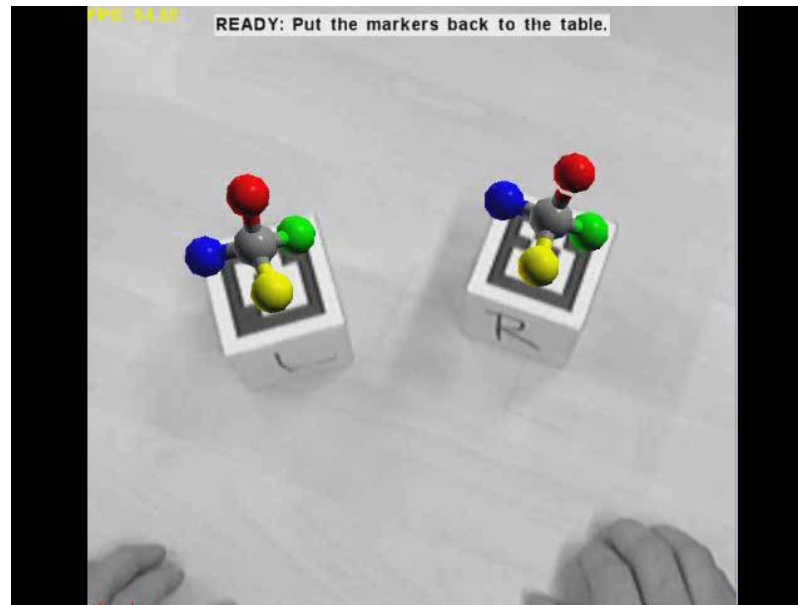
Problem: How to select a possible bond?

Approaches:

- Proximity Based
- Shake Based

Proximity Based Selection

- Freely move the molecules towards each other.
- All atoms which are able to bind and ...
- ... which are closer than a specific distance are possible binding partners.
- The shortest possible bond between these possible binding partners (atoms) is selected.



Shake Based Selection

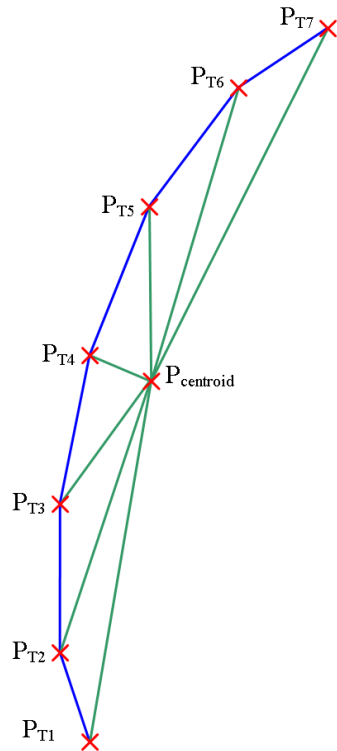
- Move the molecules towards each other
- All atoms which are able to bind and ...
- ... which are closer than a specific distance are possible binding partners.
- Perform a shaking gesture to cycle through the possible binding partners (atoms).
- The possible bond, connecting these binding partners, is selected.

→ Find a way to trigger the shaking gesture...

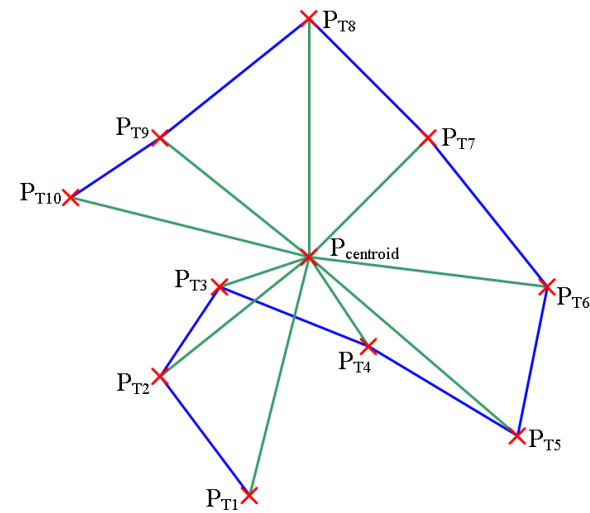


Recognition of the Shaking Gesture

Comparison of the trajectory length of the last second and its compactness:



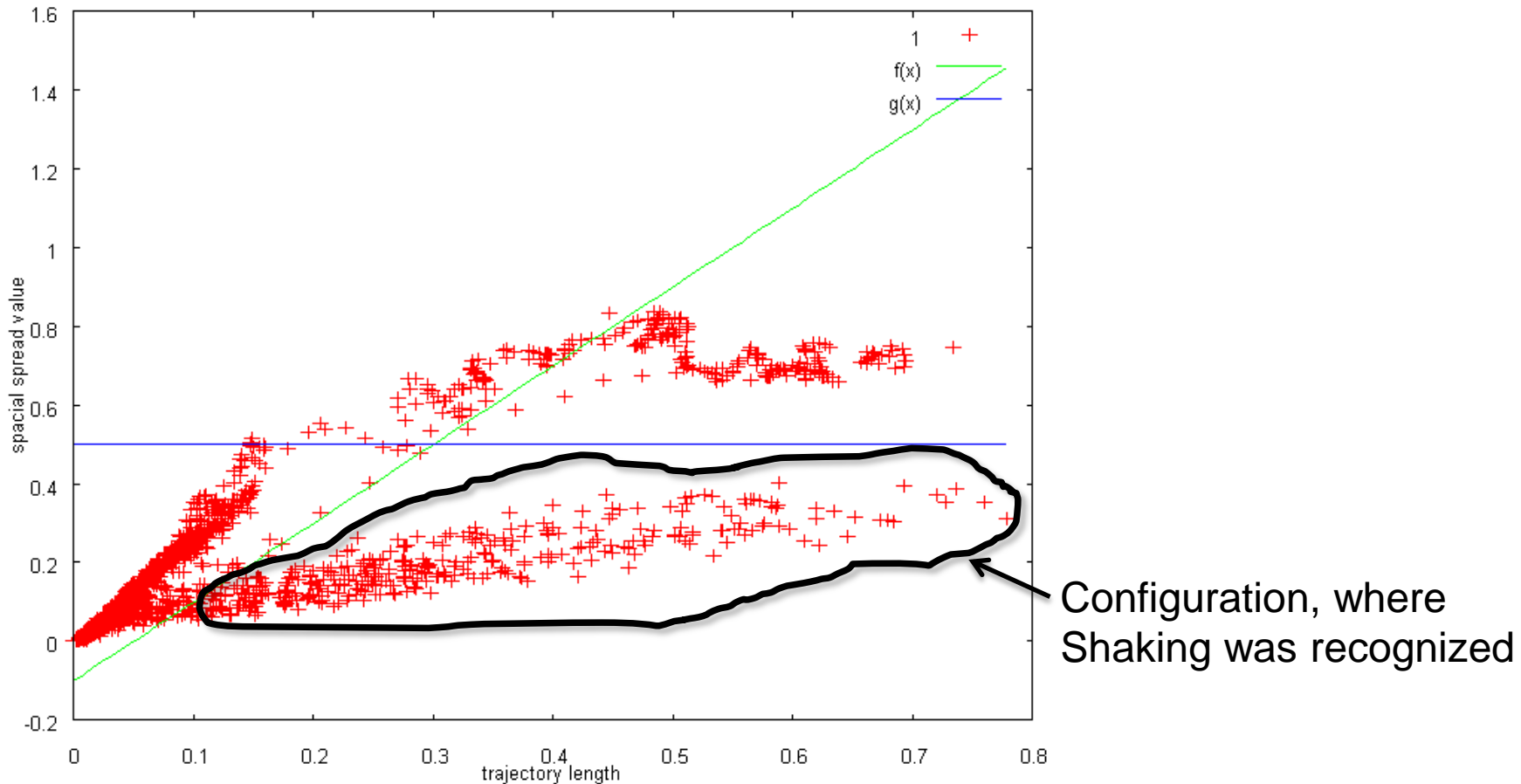
Normal Movement:
Trajectory length high and **not** compact



Shaking:
Trajectory length high but compact

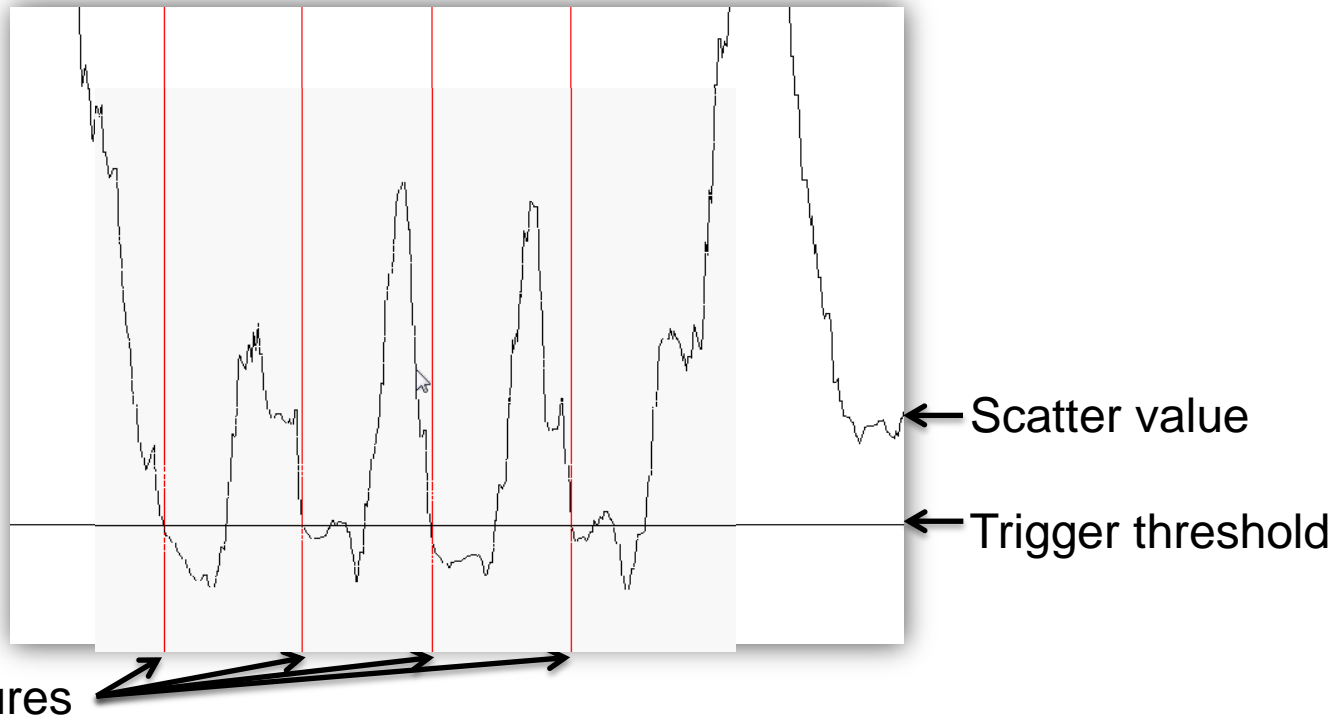
Recognition of the Shaking Gesture

- Scatterplot showing the trajectory length and the spread value (inverse compactness).



Recognition of the Shaking Gesture

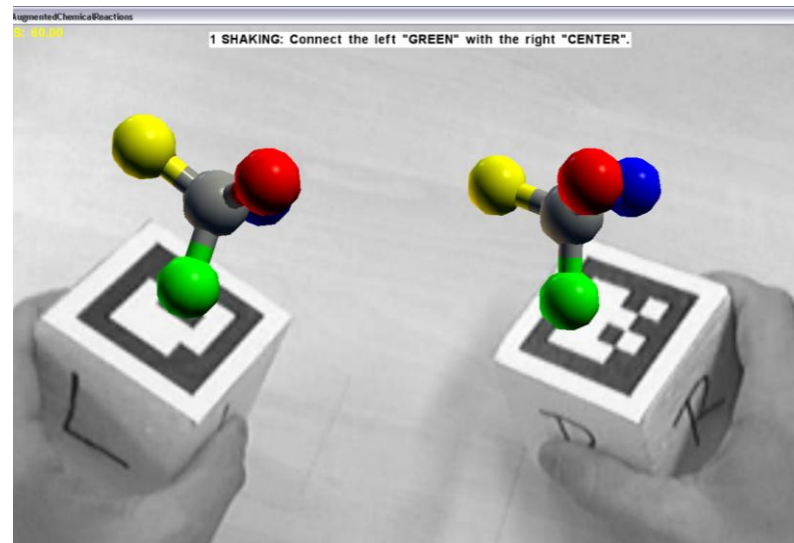
- Dynamic hysteresis to prevent multiple triggering.
- Moving hysteresis window
 - Scatter value goes below lower window boundaries → window lowers
 - Scatter value goes above upper window boundaries → window raises
- Only trigger again, when the window was raised after a triggered event.



User Study

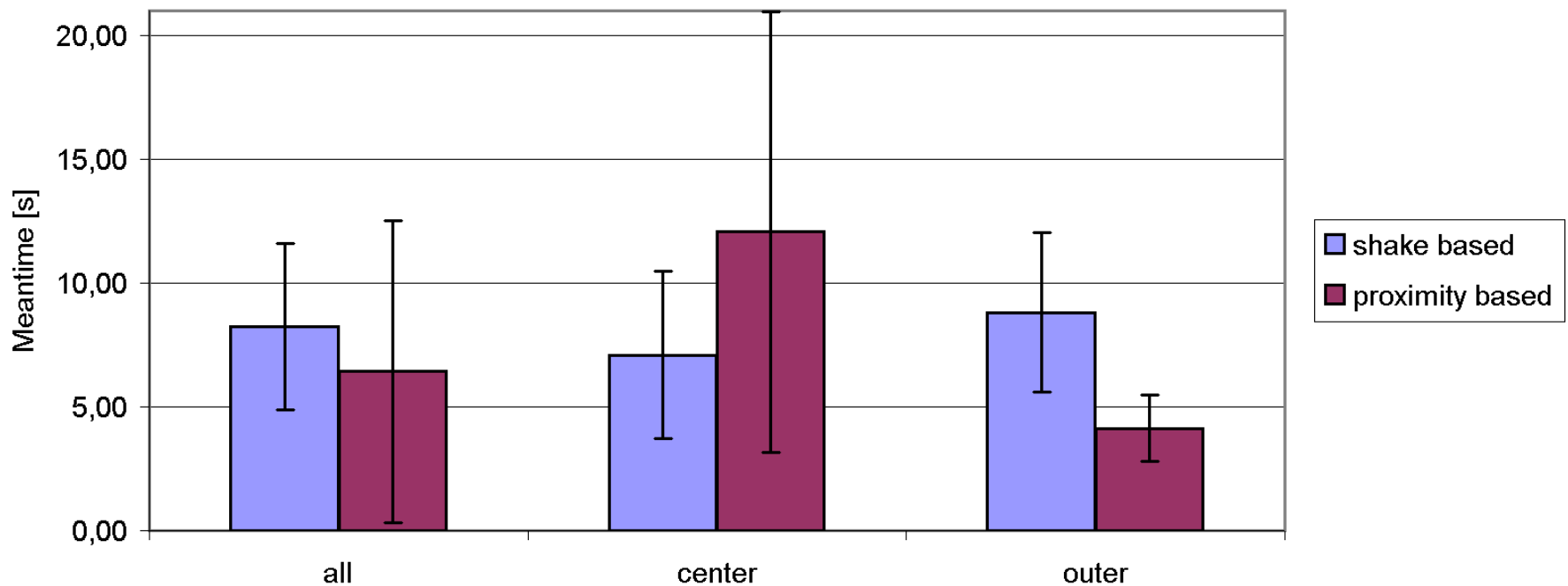
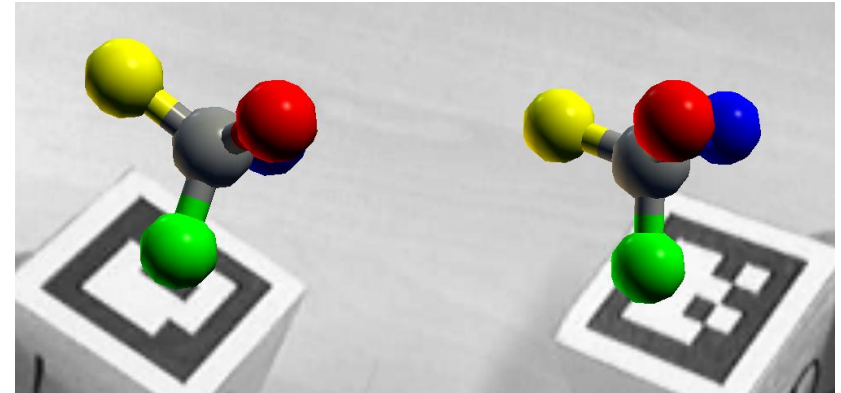
- Task:
 - Within-subject, repeated measures single-session design.
 - 19 Users (7 female, 12 male)
 - Select possible bonds which are given by the application
 - 24 combinations to select with proximity based selection
 - 24 combinations to select with shake based selection

- How fast are both methods?
- How accurate are they?



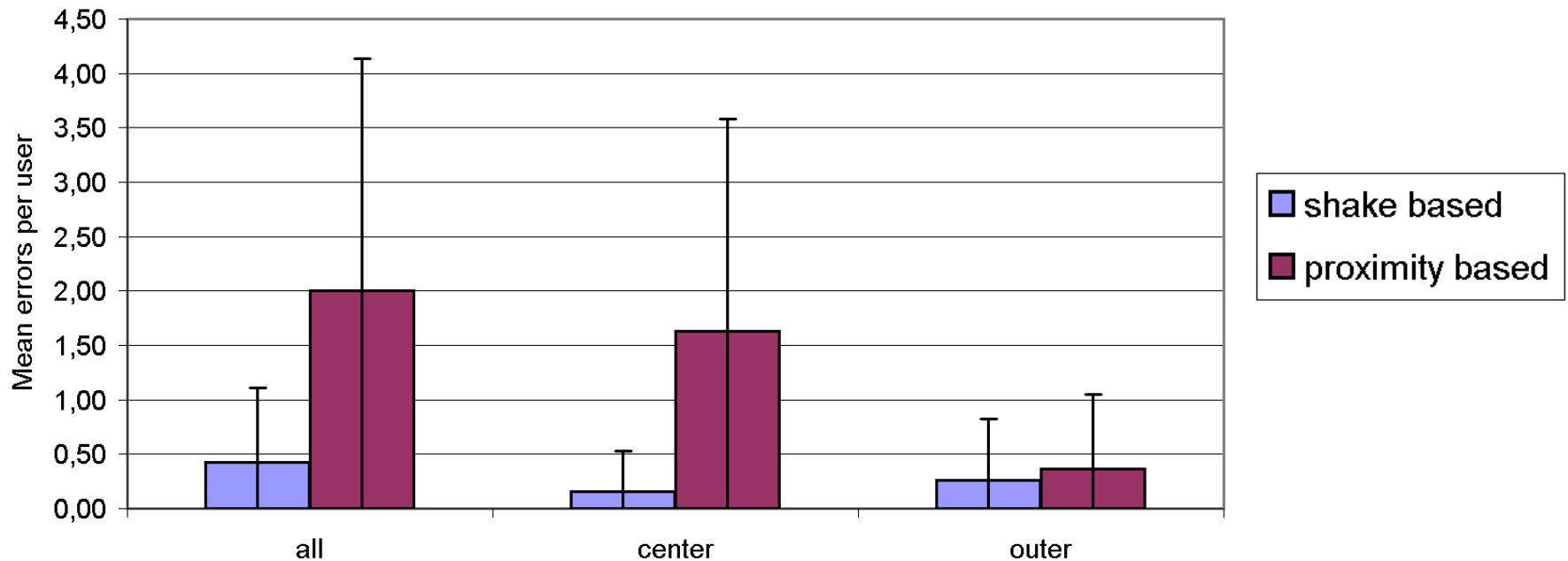
User Study – Measure Speed

- Differentiate combinations between:
 - **all** atoms
 - atoms and a **center** atom
 - only **outer** atoms
- Proximity based is faster, except for combinations with center atom.



User Study – Accuracy

- More errors with proximity based method
- Except combinations with only outer atoms



Conclusion & Future Work

Both methods have their pros and cons:

- Proximity based method:
 - is fast and easy on combinations with only outer atoms.
 - is difficult and frustrating with combinations with center atom.
- Shake based method:
 - is accurate in selecting the desired bond,
 - but slow.

Future Work:

- Combine both methods to get speed and accuracy,
- by introducing layers (like shells), and switching layers by shaking,
- Use proximity based method to select bonds from the selected layers
- Find ways to confirm the selection and connect the molecules.

Another solution:

When two hands are not enough... ask someone to help you :-)

Thank You