

Quantum Mechanics in Biological Systems with Advanced Algorithmic Methods

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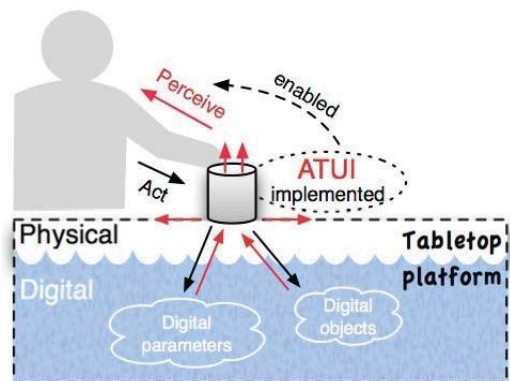
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LW WKURXJK SK\VLFDO PDQLSXODWRQV E\ KDYLQJ
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,,78,\$1'\$5

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WKH OHYHO RI LPPHUVLRQ DQG VHQVDWLRQ RI
WKH LQWHUDFWLYH SURFHVV \$ MXYHQLOLW\ \$
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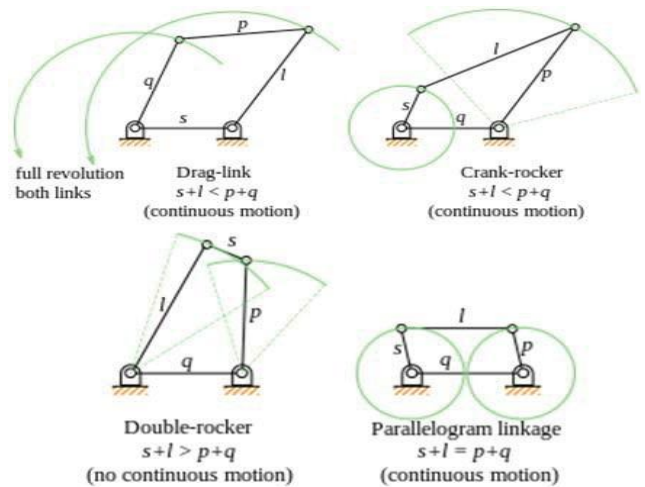
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A. Understanding the Concept of 4BL Mechanisms Problem

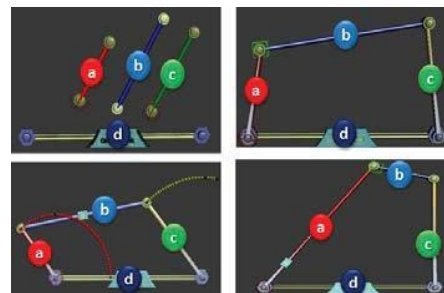
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WKHVXEMHFVWRWKH%/ZKLFKUHTXLUHVWRWRIY
LVXDOLJWLRQ
DQGLPDJLQDWRQ



B. Designing the Mechanism Using 3D Max

RIWKH%/PHFKDQLV,WDOORZVWKHXVHUVWRYLVXD
OLJHGLIHHUHQW
W\SHVRIWKHPHFKDQLV&UDQN5RFNHU"RXEOH5RFN
HU'UDJ
/LQNDQG3DUDOOHORJUDP/LQNDJH
7KH VLPXODWLRQ FDQ SURYLG WKH XVHU ZLWK
VLPXODWLRQ
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SULPLWLYHV DW WKHLU JLYHQ SLYRW
SRLQW



)LJ/LQNDJH3DUWVE'UDJ/LQNF'RXEOH5RFNHUG
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WKH&UDQN

5RFNHU

C. Developing the AR Scenes

\$Q \$5 DSSOLFDWLRQ KDV EHHQ GHYHORSHG DW
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WKH VLPXODWHG PRGHOVEXW DOVR WR
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YHORSPHQWSURFHVV
RIWKHDSSOLFDWLRQ

)LJ1HZLQWHUDFWLYH%RRNZLWKPXOWLSOHIXQFWLR
QVWRXFKLQWHUIDFH

D. Developing a Programmable Design

Before the simulation start 7KH JHRPHWULHV DQG

2. The analytical information is:

x \$QJOHRIURWDWLRQ□□DQG□
x0D[LXPDPDQGLQXPYPDOXHVRUHFDFKDQJOHUVX
OWLQJ
IURPWKHOLQURWDWLRQV

3The 4BL equations have to be solved

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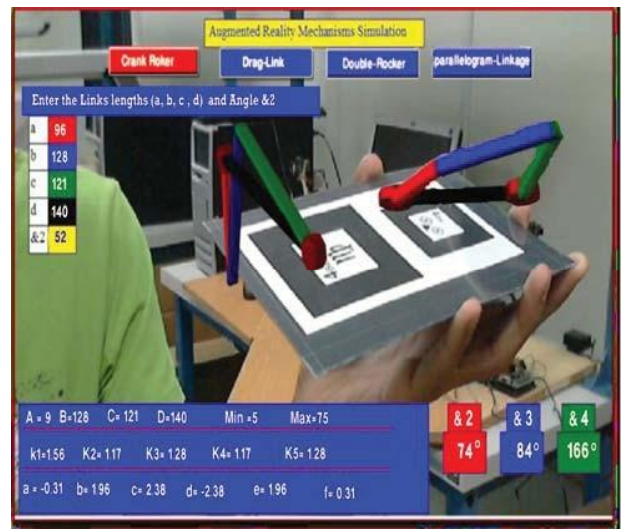
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WKHFRUUHFWSRVLWLRQVDQGDWWLWXGHV

For the interactive action, WKH V\WHP FRQWDLQV WZR

PDUNHUVWKHILUVWPDUNHUZDVXVHGWRYLHZWK
H'YLUWXDO REMHFW RI WKH %/ DQG WKH VHFROG
ZDV XVHG DV DQ

LQWHUDFWLYHNN\WRVWUWUWVRSWKHURW
DWLRQRIWKHYLUWXDO
PRGHODWDQ\WLPDVLQ)LJ7KLVFDQKHOSOHDU
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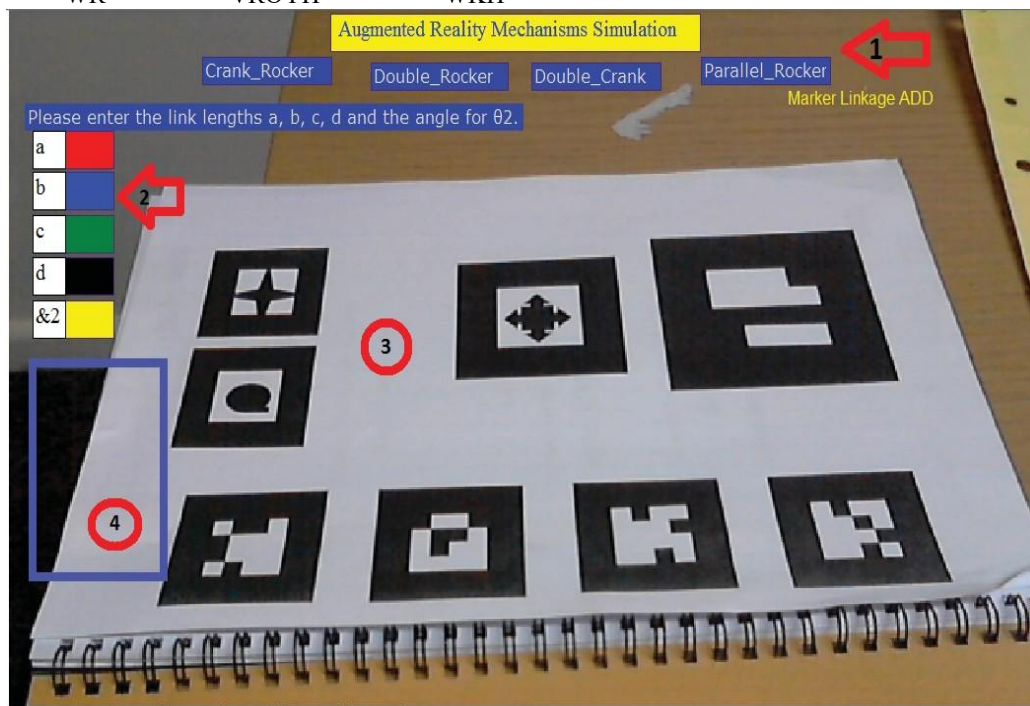
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E. Enhancing TUI with AR Design

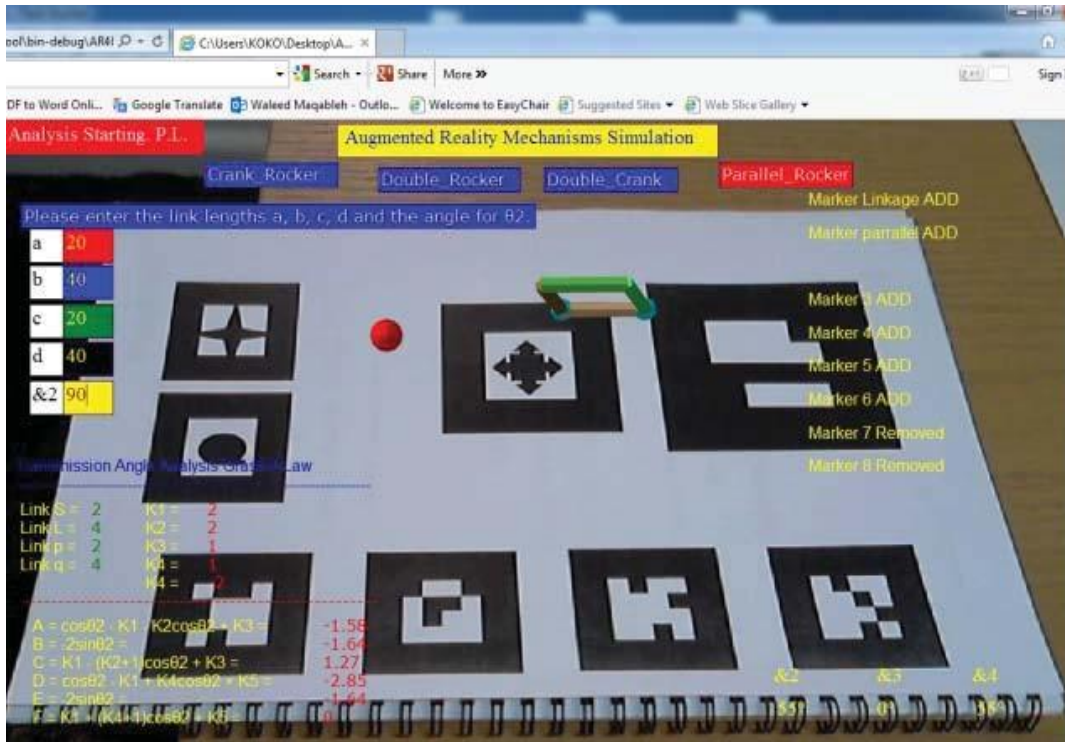
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LPSOHPHQW WKH VFUHHQ FRPSRQHVV VLQFH LW
LV FRQLGHUHG WKDW WKH *8, FDQSURYLGH

QDWXUDO DQG HDV\ PHDQV IRU XVHUV WR
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LRQ
RI WKH OLQNDJH DQG WKH DQDO\VLV VHFWRQ
VKRZV WKHUHO WLP
VLPXODWLRQSDUDPHWHUV
7KH \$5%0\$67 DSSOLFDWLRQ VXSSRUWHG E\ *8,
DQG 78, JLYHV WKH XVHUV WKH DELOLW\ WR
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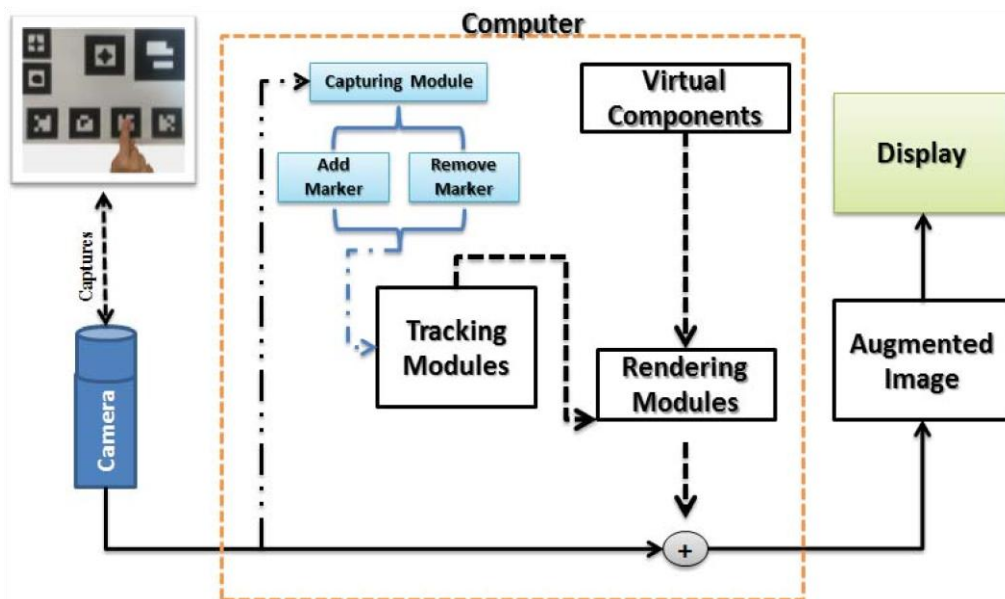
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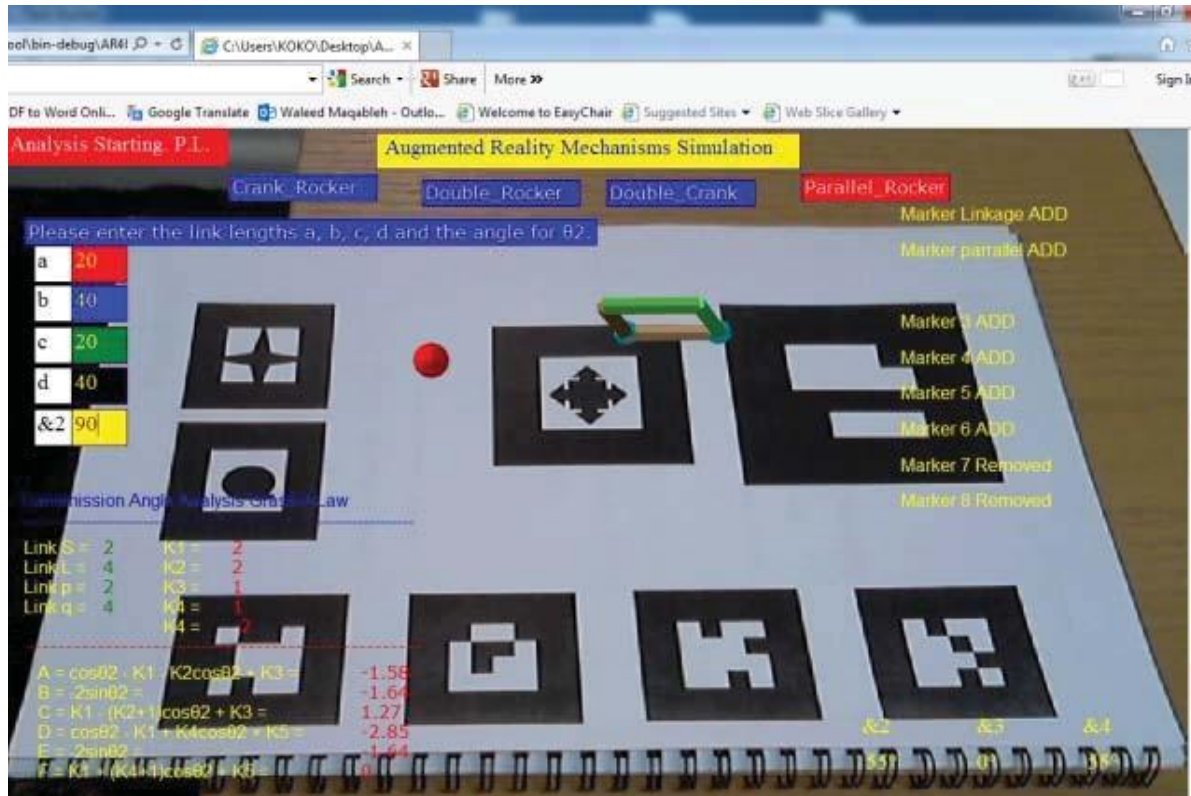
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)LJ3LSHOLQHIORZFKDUWRIWKHDSSOLFDWLRQ



)LJ7KHQHZPXOWLSOHIXQFWLRQVXVHULQWHUIDFHZLWKHLJKWWRXFKWRSULQWLQW
HUDFWLYHIXQFWLRQV

F.Evaluations of All Phases

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FDWLRQ

,95(68/76\$1",6&866,21

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)IURPWKHVFRUHVRIWKHTXHVWLRQDQGWKHUHV XOWV VKRZ WKDW WKHUH LV D SRVLWLYH LPSDFW RI WKH DSSOLFDWLRQ SRWHQWLDQV LQ LPSURYLQJ WKH VWXGHQW XQGHUVWDQGLQJ RI WKH

EHKDYLRURIWKH%/PHFKDQLVP)RUH[DPSOHWKHGD
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 WKH VWXGHQW WR FDKQJH WKH
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 VWXGHQWV WKH DELOLW\ WR YLVXDOL]H
 GLIIHUHQW W\SHV RI WKH %/ ZKLOH WKH PHFKDQLVP
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 WKH PHFKDQLVPWRFKDQJHLWVW\SH
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7KHVLPXODWHGSDUDPHWHUVDPNHLWHDV\WRLGH
 QWLI
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