CALIBURN:

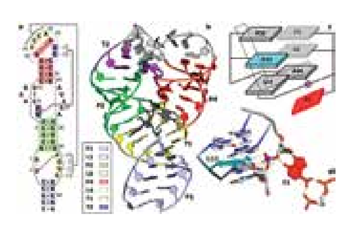
ADVANCED CYBERINFRASTRUCTURE REPORT

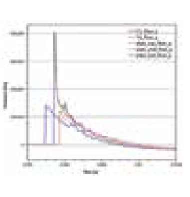
Rutgers Discovery Informatics Institute: Accelerating discovery in the State of New Jersey through high performance computing

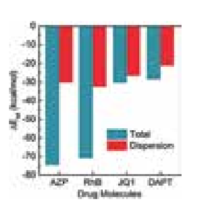
RUTGERS
THE STATE UNIVERSITY
OF NEW JERSEY

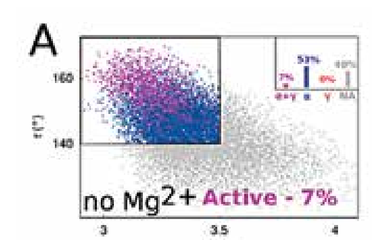
JUNE 2019

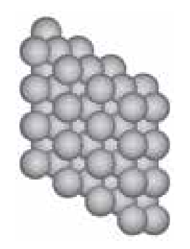

1-Azakenpaullone

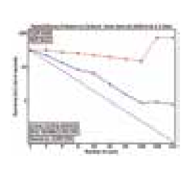


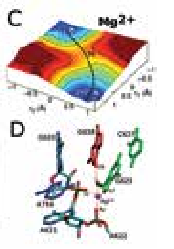


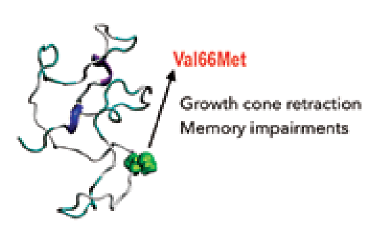

0
-10
-20
-30
-40
-50
-60
-70
-80
ΔG_bd (kcal/mol)
Total
Dispersion
AZP
RhB
JQ1
DAPT
Drug Molecules

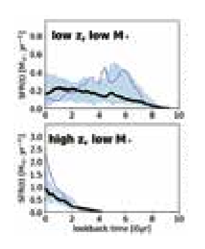

A
160
140
τ (°)
53%
7%
6%
40%
α+γ
β
γ
NA
no Mg2+
Active - 7%
3
3.5
4
r (Å)

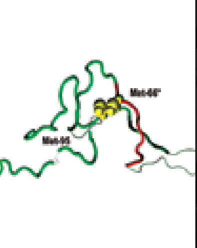


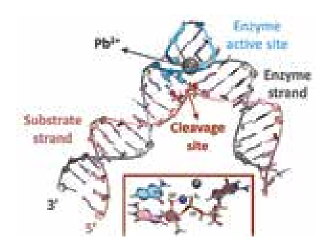


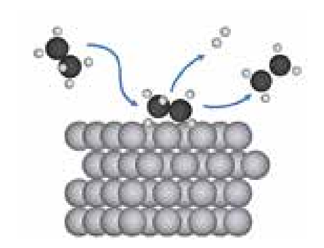

C
Mg2+
D

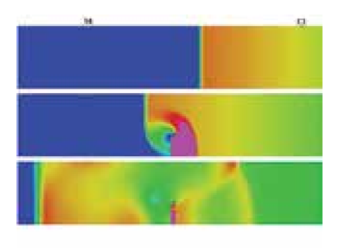

Val66Met
Growth cone retraction
Memory impairments

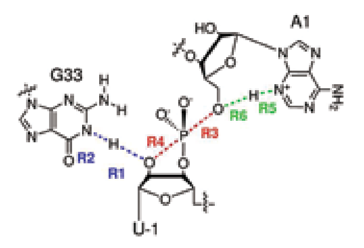

low z, low M*
high z, low M*
lookback time [Gyr]

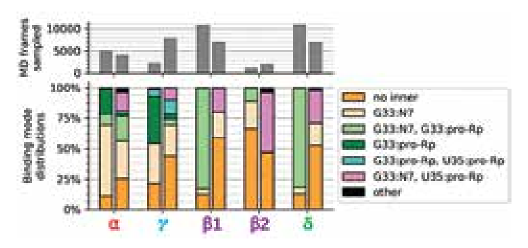

Met-66
Met-95

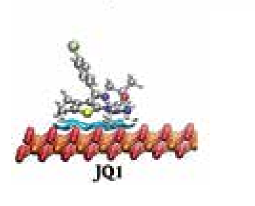

Pb2+
Enzyme active site
Enzyme strand
Substrate strand
Cleavage site
3'
5'

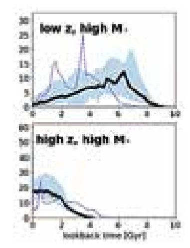


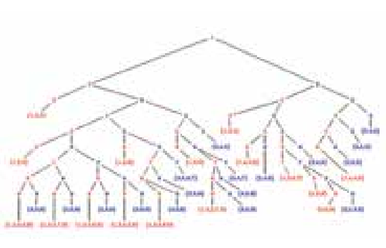


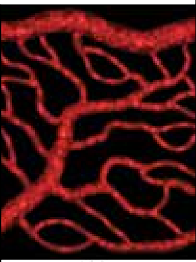

HO
A1
G33
R4
R3
R6
R5
R2
R1
U-1

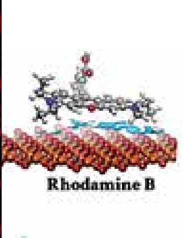

MD frames sampled
10000
5000
0
Binding mode distributions
100%
75%
50%
25%
0%
no inner
G33:N7
G33:N7, G33:pro-Rp
G33:pro-Rp
G33:pro-Rp, U35:pro-Rp
G33:N7, U35:pro-Rp
other
α
γ
β1
β2
δ

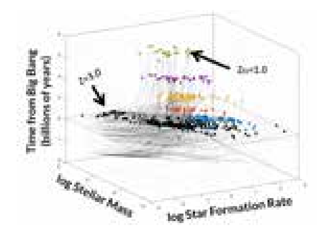

JQ1

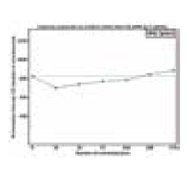

low z, high M*
high z, high M*
lookback time [Gyr]

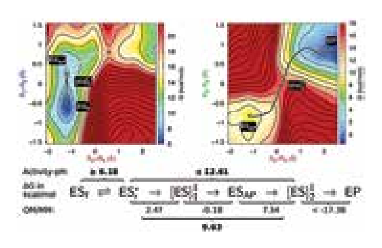


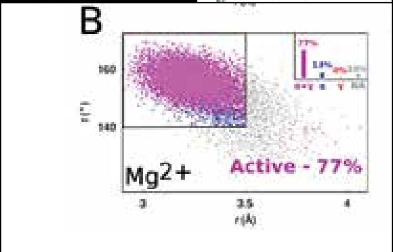


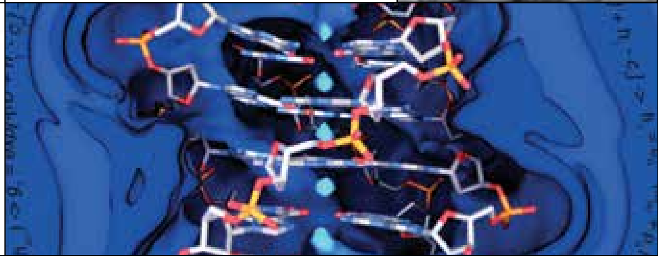

Rhodamine B

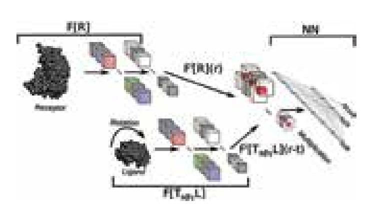

Time from Big Bang (billions of years)
z=3.0
z=1.0
log Stellar Mass
log Star Formation Rate

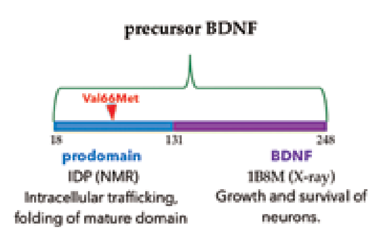


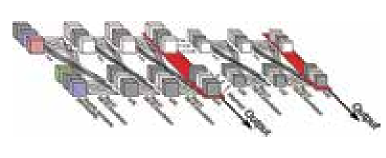

Activity-pH
≥ 6.18
≤ 12.61
ΔG in kcal/mol
ES_I
ES*
EP
QM/MM:
2.43
-0.18
7.34
≤ -17.36
9.43

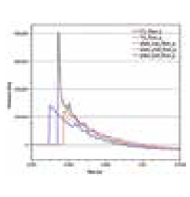

B
160
140
τ (°)
77%
18%
4%
3.6%
α+γ
β
γ
NA
Mg2+
Active - 77%
3
3.5
4
r (Å)

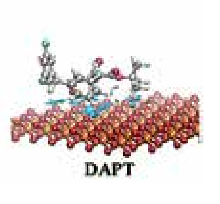


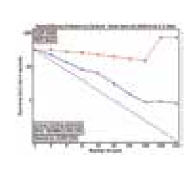

F[R]
NN
Receptor
F[R](r)
Rotation
Ligand
F[T_αβγL](r-t)
F[T_αβγL]

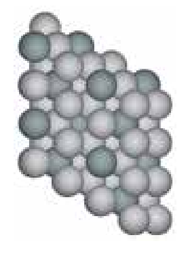

precursor BDNF
Val66Met
18
131
248
prodomain
IDP (NMR)
Intracellular trafficking, folding of mature domain
BDNF
1B8M (X-ray)
Growth and survival of neurons.

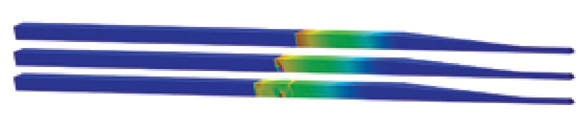

Output
Output

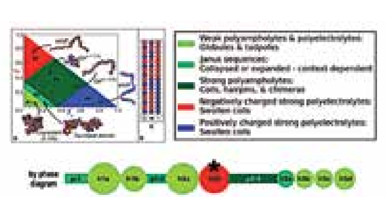


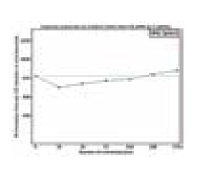

DAPT

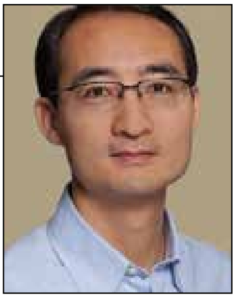







Weak polyampholytes & polyelectrolytes: Globules & tadpoles
Janus sequences: Collapsed or expanded - context dependent
Strong polyampholytes: Coils, hairpins, & chimeras
Negatively charged strong polyelectrolytes: Swollen coils
Positively charged strong polyelectrolytes: Swollen coils
by phase diagram





High Fidelity Simulations of Shock Wave Reflection Inside a Shock Tube

PI: Xianlian Alex Zhou, PhD
Institution: New Jersey Institute of Technology, Department of Biomedical Engineering

EXECUTIVE SUMMARY:

Exposure to blast waves is the leading cause of Traumatic Brain Injury (TBI) in military personnel. Many studies, both experimental and numerical ones, have been conducted to investigate the cause of TBI due to primary blast overpressure. Shock tubes are the main laboratory tools for generating blast-like shock waves traveling along a long chamber, within which different objects (such as animal or human phantoms and live animals such as rats) can be stationed and the overpressure reflected from and transmitted into the objects can be monitored. The Shock Wave Testing Facility at the Center of Injury Biomechanics, Materials, and Medicine (CIBM3) of New Jersey Institute of Technology (NJIT) has installed two square cross section shock tubes: one is 9″ wide and the other is 28″ wide, and both are longer than 6 meters. Work has been done to adjust and calibrate the shock tubes to generate pure, primary shock waves similar to that from field blasts. Currently, an ongoing effort has been carried out to investigate the reflection wave from objects placed inside the shock tubes. Plate objects with different sizes and material properties (e.g. aluminum vs plastic) have been tested and the pressure data on incident and reflection waves have been collected. To better understand and analyze the experimental data collected, we have been using modeling studies to reproduce some of the phenomenon observed and to reveal how sizes and materials affected the wave reflection. The findings will have profound impacts on how the shock wave shall be modeled correctly and accurately with data validation and how objects of different sizes and materials (rat vs human, phantom vs live tissue) could impact the wave reflection and transmission. And we expect this study will greatly help us to better understand TBI primary injury mechanism and continue to push the state-of-the-art in TBI research.

RESEARCH CHALLENGE:

There are several challenges in modeling shock wave traveling inside shock tubes with CFD (Computational Fluid Dynamics) and FSI (Fluid Structure Interaction) simulations. To capture the shock front with steep pressure gradient, very small cells must be used to obtain reasonable accuracy. Considering the length scale of the square shock tubes (>6m), the computational grid can easily exceed several million cells. In addition, a very small timestep, around the scale of 1μs (microsecond) or less, shall be used for transient/dynamic analyses. To simulate over 20ms of shock wave generation and propagation, typical workstation computers or even small clusters can take weeks or longer to complete just one simulation. Our goal is to conduct parametric simulations to cover most of the experimental conditions (different incident pressures and different objects). Consequently, high performance computing cluster resources are required.

METHODS AND CODES:

Simulations of shock wave reflection from an aluminum plate placed inside the 9″ shock tube were conducted with an in-house multiphysics FSI solver that is written in C++ and uses MPI for parallel computation. The high-pressure chamber (at the right narrower end of Figure 1(a)) contains a mixture of helium and air whereas the square tube and the tapped transition region are filled with air at the atmospheric pressure. The square aluminum plate has a width of 3″ and a thickness of 0.34″ and is positioned in the middle of the square tube. Due to symmetry, only a quarter of the shock tube was modeled as shown in Figure 1(a). The mixture flow was solved with a finite volume based CFD solver and the deformation of the aluminum (linear elastic) plate was solved with a finite element solver. These two solvers were strongly coupled and iterated to achieve convergence during each time step.

RESULTS:

The FSI simulation of shock wave reflection solves several field variables, including the mass ratios of helium and air, flow pressure and temperature, as well as the deformation and stress of the plate. Many monitor points were placed inside the simulation domain to monitor the profiles of these variables. For example, the monitor point C1 is located on the top of the tube and in front of the plate; T4 is located behind the plate, as shown in Figure 1(b); and three monitor points are placed along the diagonal line of the plate. These monitor points are positioned at the same locations of pressure sensors employed in the experiments for model validation purpose. Figure 1(a-b) shows the pressure fields inside the shock tube at three different time steps right before and after the reflection, and Figure 1(c) shows the pressure profiles of the 5 monitor points for a 12ms duration. The reflected pressures on the plate are almost three times that of the incident pressure at C1. And the durations of positive pressure phases are between 4 to 5ms. These simulations provide the data needed for model calibration and cross-validation of experimental measurements and simulation methods and results. Additional simulations with plates of different materials and thicknesses can provide clues on how the pressure or impulse can be attenuated by the plates and if a plate of chosen material can be effective in reducing pressure and protecting structures behind it. Through such a model validation study, we can gain confidence in applying this computational method to simulate the complex phenomenon of TBI with helmet protection. The predicted blast overpressure and positive pressure impulse (integral of pressure in time domain) are highly relevant indicators of potential TBI risks for people who sustained blast overpressure. Future work can be conducted to evaluate and design helmets with high efficacy in TBI protection.

ROLE OF CALIBURN AND RDI²:

The Caliburn cluster of RDI² has cutting edge hardware and software for high performance computing. And the staff at RDI² provided the expertise, help, and support we needed to conduct our simulations. It enables us to continue parametric simulations of shock wave reflection with different plate dimensions and materials and even totally different objects.

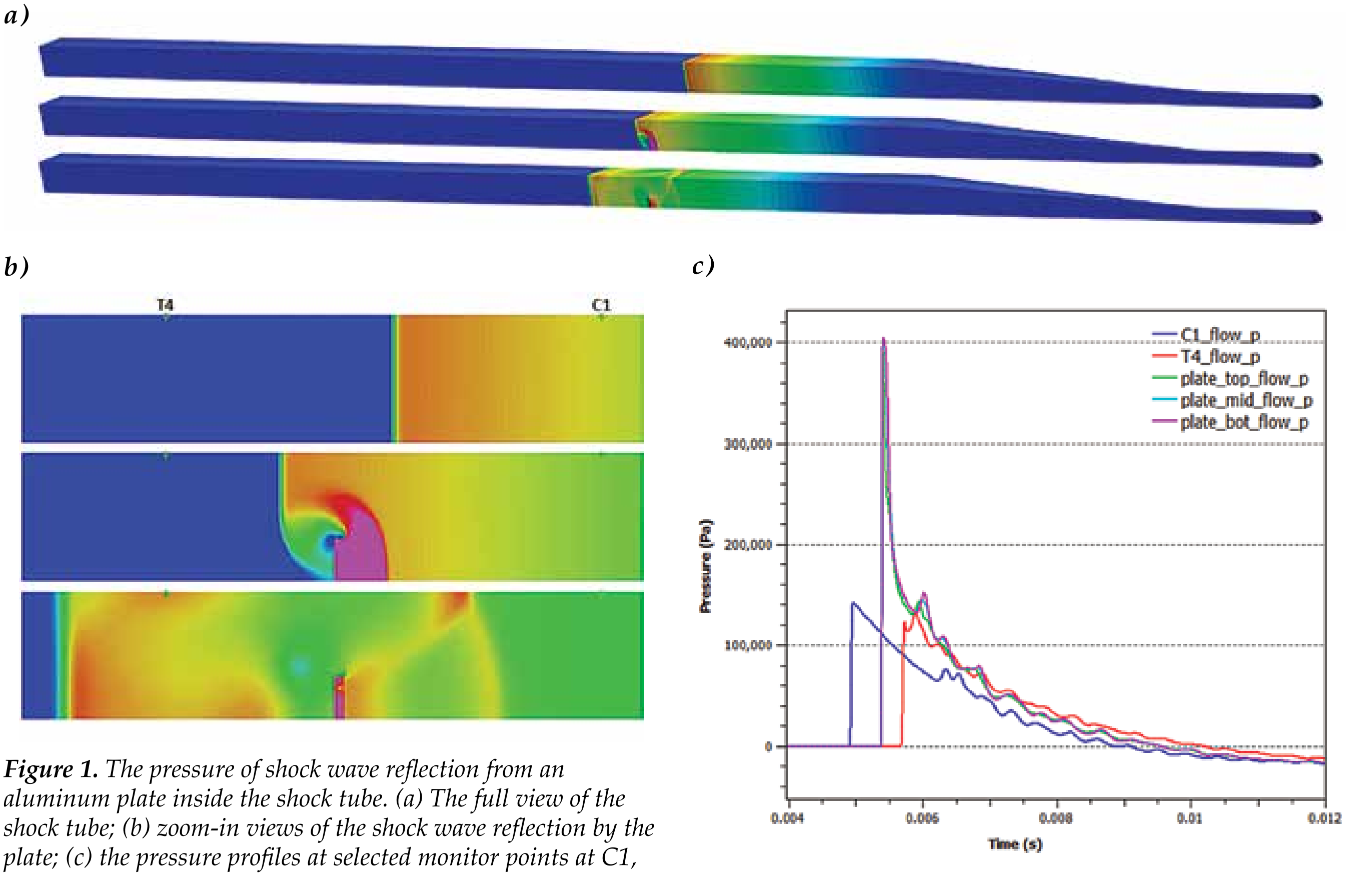


Figure 1. *The pressure of shock wave reflection from an aluminum plate inside the shock tube. (a) The full view of the shock tube; (b) zoom-in views of the shock wave reflection by the plate; (c) the pressure profiles at selected monitor points at C1, T4, and three locations on the plate.*

This publication was designed and produced by the Rutgers Discovery Informatics Institute (RDI^2), a division of the Office of Research and Economic Development at Rutgers University. RDI^2 extends its thanks to the research teams who contributed summaries of their latest Caliburn enabled research for inclusion in this report. Caliburn is supported by the State of New Jersey and Rutgers University.

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