VRシミュレーションシステム
VR Simulation System

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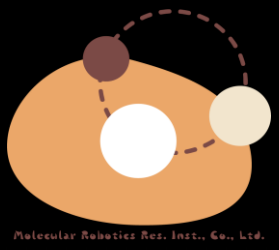


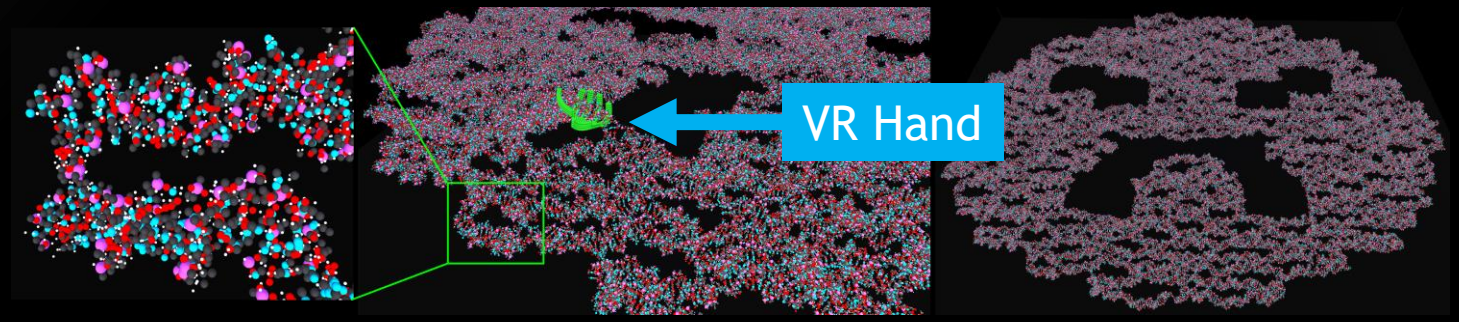
Computing Background

Greg Gutmann

- PhD. Work: Microtubule Simulation
  - **Distributed GPGPU Simulation with Distributed Workload Balancing**
    - Near perfect scaling (~95% efficient)
    - *~10 millisecond simulation budget*
    - Tested on 10 Nvidia Titan Pascal GPU connected by PCIe

10 million particles (~2017)

- Technology Expertise:
  - GPGPU
  - Networking (sockets)
  - VR (Rendering / HCI)
  - AI (Nvidia DLI)



DNA Origami: 440,000 atoms (~2021)

VR Simulation

Tuned for molecular-molecular interactions

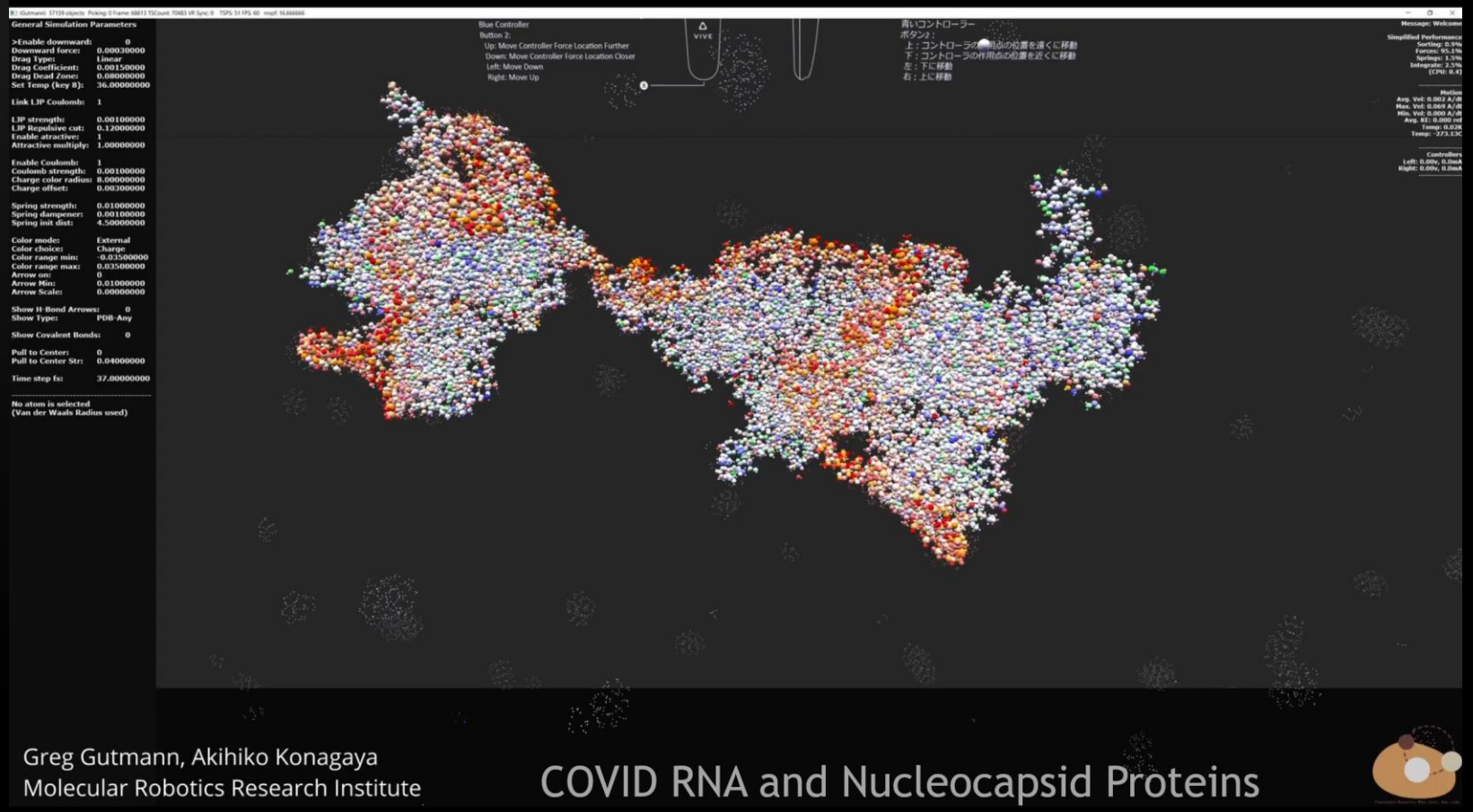
Less time needed than conventional MD methods

Example:

1. Clicked start
2. Left for lunch 30 min
3. Returned to this

The Nucleocapsid protein binds to RNA to form ribonucleoprotein (RNP) structures for packaging the genome into the viral capsid.

doi:10.1016/j.antiviral.2013.12.009
doi:10.3390/v6082991



Objectives of VR Simulation Framework

- Simulate large molecular-molecular interactions
  - To aid in the development of Molecular Robotics or other micrometer scale systems
- Enable direct interactive simulation by users [Slide 6]
  - Human-in-the-loop: User can gain a deep understanding of dynamics, while gaining results
- Enhance communication around nano to micro scale phenomenon [Slide 7]
  - Boost knowledge/interest in the work to support the research
- Create a scalable / flexible interactive VR framework [Slide 9]
  - In terms of: Cost, models, local / remote

Recent AI Models

Example: Alpha fold

- Alpha fold's purpose is the shape of proteins
  - We do use Alpha fold within our group to generate proteins to load into our simulation *(Kondo-san, Kansai University)*

- Our VR simulation's purpose is to simulate molecular-molecular interactions at a larger scale
  - *100s of thousands to over a million atom range*

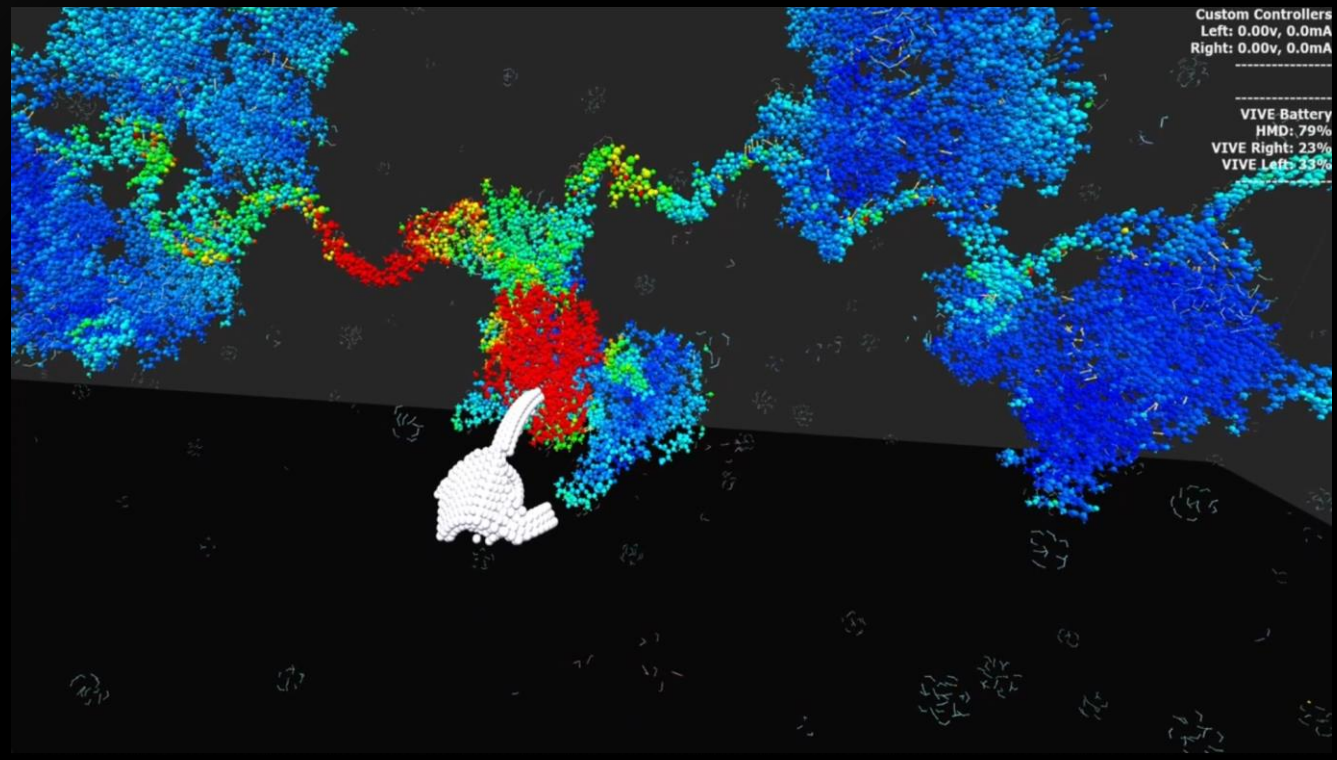
Image from Google Search

We do have interest in exploring other AI models for VR simulation, adding existing models or developing our own, to be covered in "Next Steps"

Benefits of Interactive VR simulation

A coarse-grained simulation

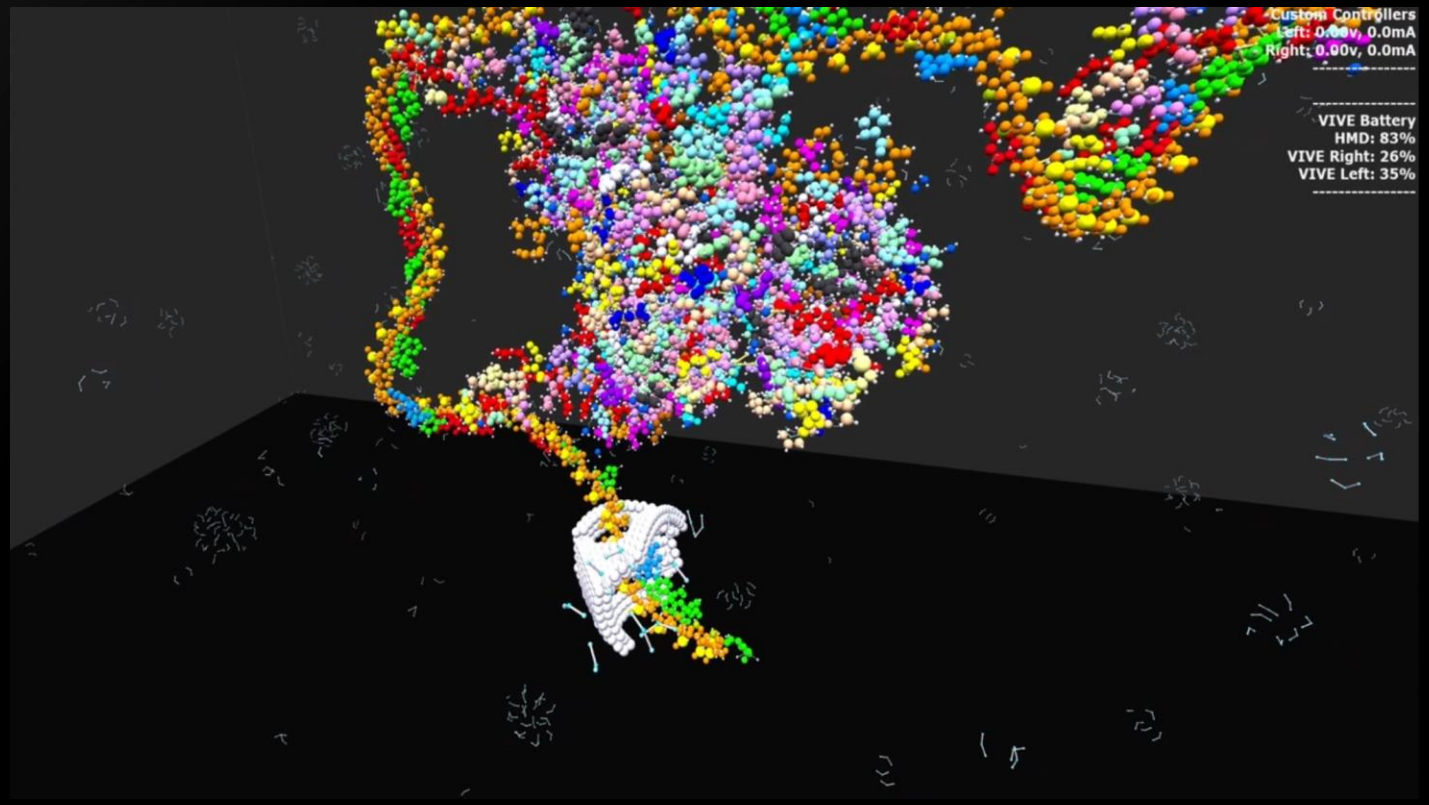
- Experiment with new ideas
  - Molecular Legos
- Visualize and test interactions
  - Electrostatic
  - Lennard-Jones
  - Hydrogen bonds
- Experiment at scales which cannot *quickly* be done with tools like MD and MO



COVID RNA and Nucleocapsid Proteins

Benefits as a Communication Tool

- Explain ideas with dynamic visual simulation
- Increase people's intuition and understanding of the nanoscale-world
- Generate more interest in your work



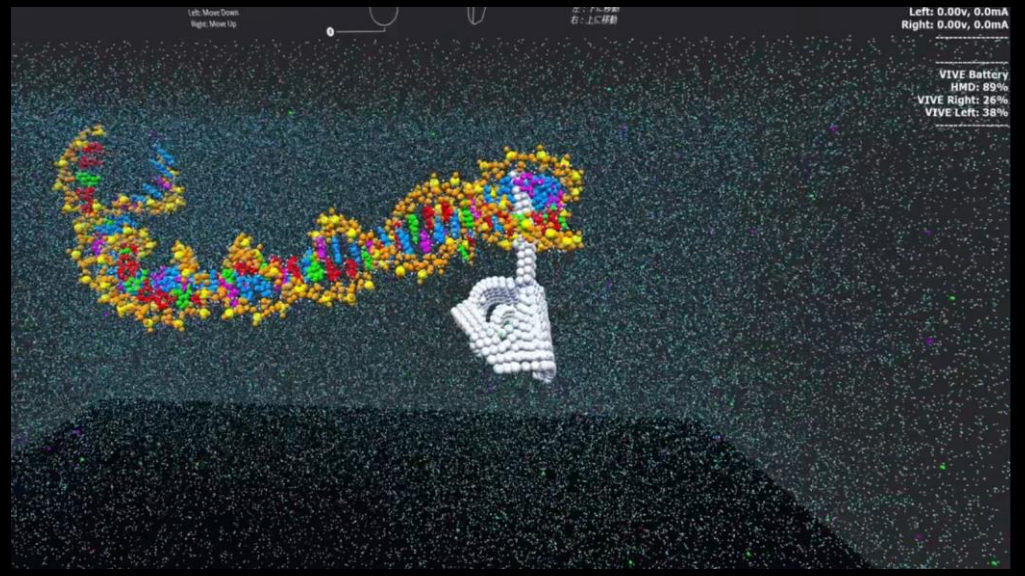
COVID RNA and Nucleocapsid Proteins

What We Have Achieved for VR

Version that is Ready for Users

Ease of access:

- Can run on a single gaming laptop



DNA in Explicit Solution

Model:

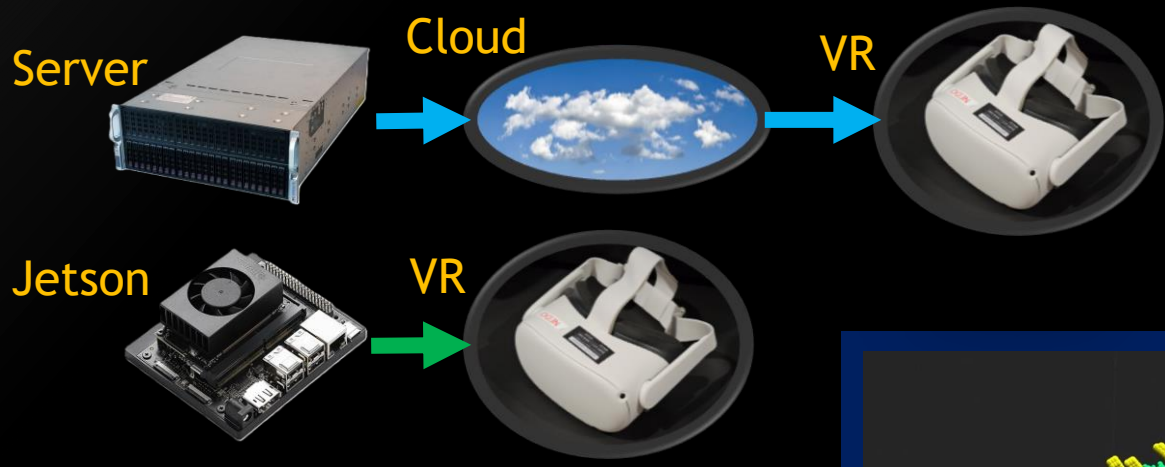
- Stable DNA strands with hydrogen bonds
- Aggregation of H2O in minor groups
- DNA can self-repair up to about 3 turns of unwinding

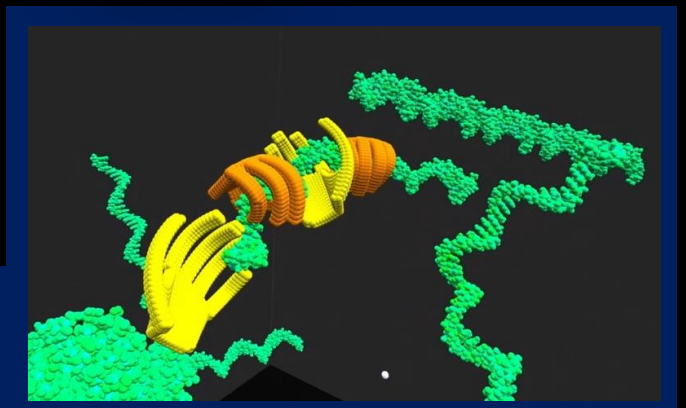
Our Computational Framework Targets

Active Prototype / Testing

A simulation framework that can:

- **Scale between:**
  - Nvidia Jetson boards
  - Personal Computers
  - Multi-GPU nodes
- **Run either:**
  - Locally
  - In the Cloud
- **Models:**
  - Ability to swap models





Collaborative Environments

Our paper: DOI: 10.1515/jib-2022-0017

Clients: Kanagawa --> Server: Sakura Internet in Hokkaido

Our Computational Framework Targets

Next Steps for Large Scale Interactive VR

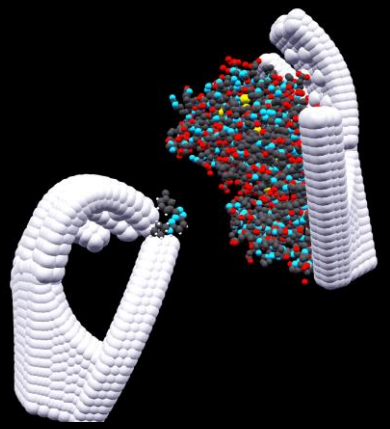
- The ability to switch between:
  - Conventional simulation and
  - **AI force fields** → As GPU hardware performance has shifted to AI operations such as Tensor cores and TF32 types
    Also, quantum effects are expected to increase stability of DNA [1]

- Challenges adapting existing AI molecular simulation:
  - *Existing solutions are fast but usually not interactive VR rates [3]*
  - *How to still visualize different aspects of the dynamics independently*
  - *Existing solutions mostly trained on only small molecules [2,3]*
    - *Solutions?: Self-Supervised, Online learning from conventional simulation [4,5]*

[1] https://pubs.acs.org/doi/abs/10.1021/ja102004b, [2] https://doi.org/10.1063/5.0007276, [3] https://www.nature.com/articles/s41586-021-03819-2, [4] doi.org/10.3390/technologies9010002, [5] doi.org/10.3389/fmolb.2021.812248

Call for Users and Feedback

- Actively looking for users for our single machine version
  - Collaborations
  - User feedback
  - End users
- Let us know how you could envision using such a platform
  - Direct usage?
  - Is there other particle like data to view?



Using Virtual Atomic Hands

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Thank You

Acknowledgements

Nishi Katsuya
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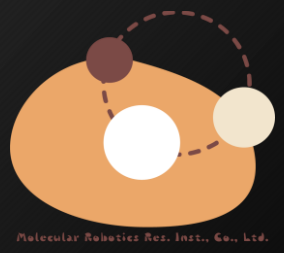

Akihiko Konagaya
Molecular Robotics Research Institute
- Venture Members
- Research labs at: Kansai Daigaku, Kyoto Daigaku, Tokyo Daigaku

https://en.molecular-robot.com/en/