

The background of the slide is a complex, colorful molecular simulation. It features a dense arrangement of spheres (atoms) in various colors including green, blue, purple, red, orange, and yellow. These spheres are connected by lines representing bonds, forming a large, irregular, and somewhat crystalline structure. A dark gray rectangular box with a thin white border is centered over the middle of the image, containing the title and authors' names.

Code-your-own iMD-VR molecular simulations

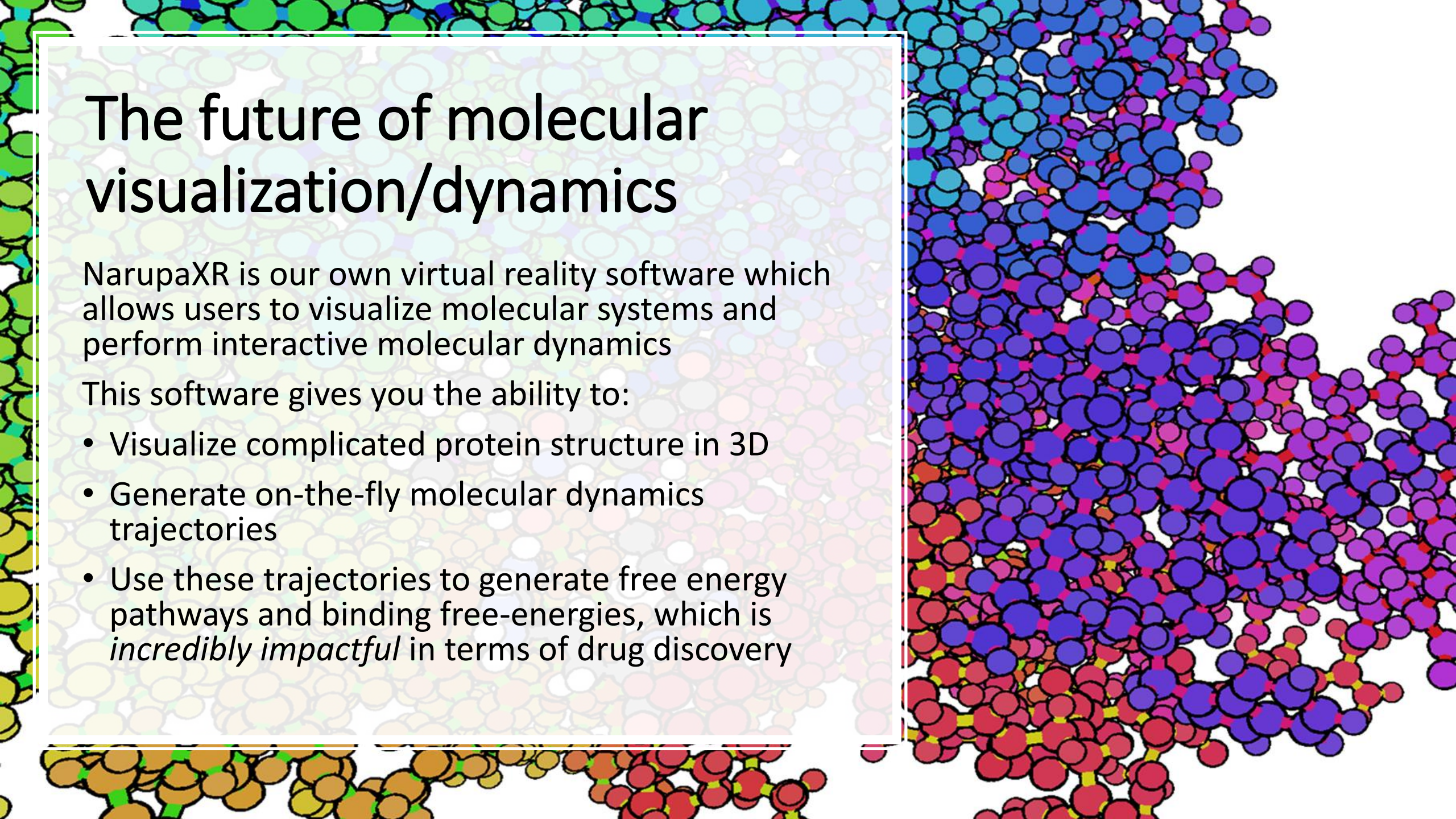
Becca Walters & Alex Jamieson-Binnie

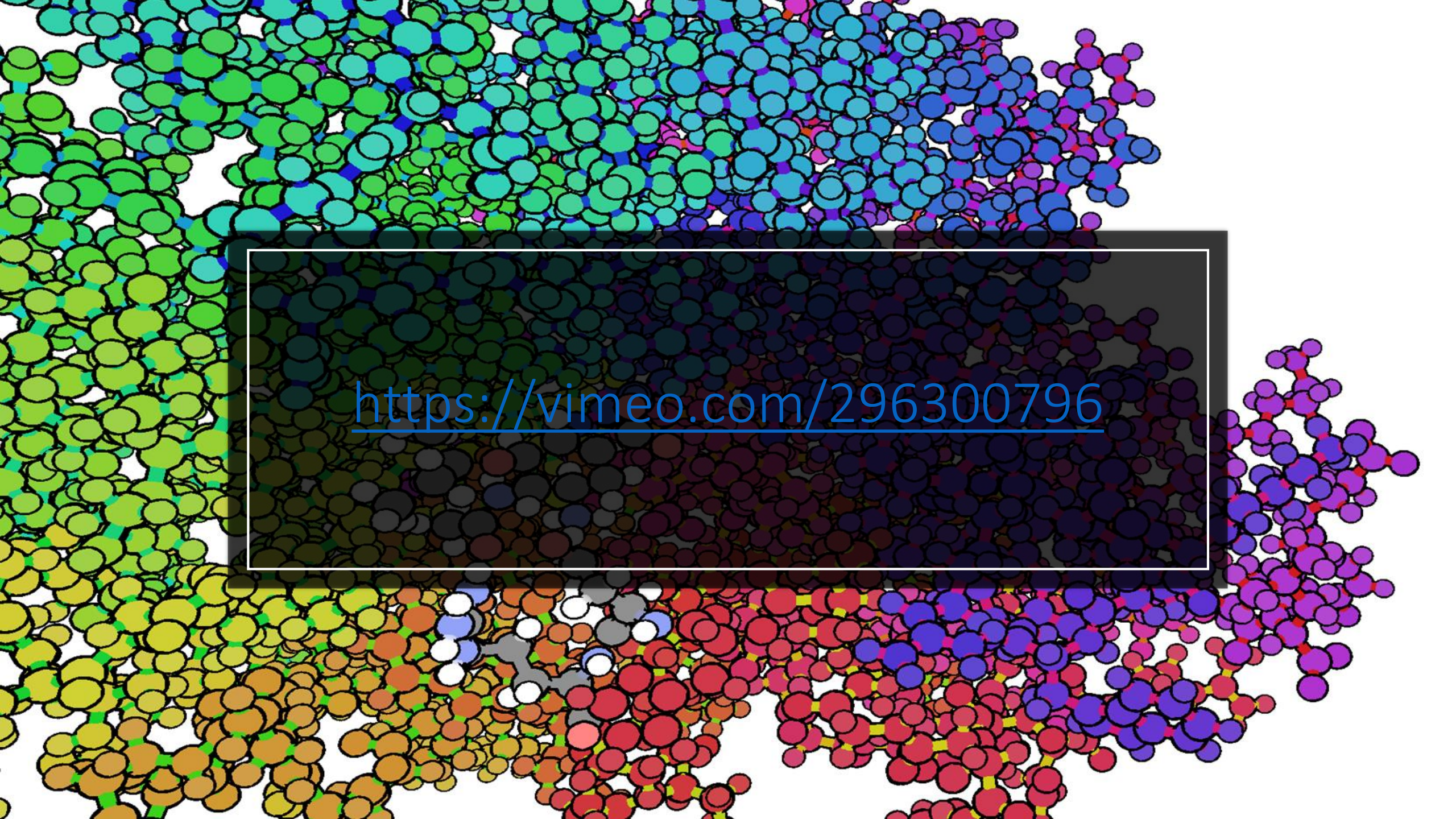
The future of molecular visualization/dynamics

NarupaXR is our own virtual reality software which allows users to visualize molecular systems and perform interactive molecular dynamics

This software gives you the ability to:

- Visualize complicated protein structure in 3D
- Generate on-the-fly molecular dynamics trajectories
- Use these trajectories to generate free energy pathways and binding free-energies, which is *incredibly impactful* in terms of drug discovery





<https://vimeo.com/296300796>

You will have the opportunity to:

- Parameterise a protein-drug system (influenza protein and Tamiflu)
- Write a python script that transforms the system into a VR simulation
- Manipulate your chosen protein in VR
- Edit your scripts to optimize the output you get from VR
- Show and tell!

