

3DVC_Friday_Infrastructure

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Infrastructure group:

Been to meetings like this. A lot of technological solutions to many problems already exist, some are 20 years old. Part of it putting it altogether is sociological. There are also sociological aspect in this aspect.

Many different user groups, and many different tools, how to identify the state of where we are.

High school student named mars rover "curiosity". "persistence". Two traits of scientists.

What problems can we solve that we have not solved? Cells in its entirety à cell biology.

Systems biology has no spatiality. Important for the 3D aspect.

Off target of drugs. Computational toxicology.

Where are the baby steps that we can take? In the earthquake example, different groups working on different things, and take 5 to 8 years to integrate different models.

Mcell took 27 years to develop. Some predictions are experimentally validated. There has to be long term commitment to tools development.

Subcellular localization of things are very contentious. Where is everything located? Can we represent knowledge using a 3D cell framework?

What happens when I change some conditions and why? Can we run the virtual experiment before wet lab? When we have the models, it is possible to predict results that experimentalists are trying to solve.

Digital experiments are difficult to reproduce, identifying the parameters used for different solutions.

For proteins in the PDB, you can visualize the atoms in different ways, and can be used as input in different experiments. You may be able to build simulations of complex environment. Just with structures, you can do many things. If we scale the concept of the PDB, and show all the parts of the cell, as in the example of G. Johnson, cellpack. That's already very exciting.

Reproducibility, replicability, or inspectability?

Virtual witnessing, Steven Shafen?— Robert Hook did experiments, publish in Royal Society Transactions, other people may see that. "Show me how it's done", in a "3D virtual cell theatre".