NEURON for multiscale simulations: reaction-diffusion and electrophysiology

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Introduction

- NEURON is widely used for simulating electrophysiology.
- NEURON 7.3 included a module for reaction-diffusion simulation, to facilitate the study of chemical-electrical interactions.
- Current work includes expanding reaction-diffusion capabilities and interfacing different techniques.
- Model specification is independent of discretization or solver.

Plugins

To support functionality not yet implemented in NEURON and domain-specific solvers, we are developing a plugin framework. Plugins must provide:

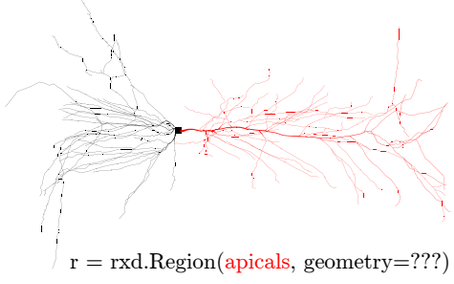
- sol.init(species, reactions)
- sol.advance(dt)
- sol.set_rate_of_change(nodelist, values)
- sol.transfer_states_to_neuron(which=None)
- sol.transfer_states_from_neuron()
- sol.supported_sim()

Activate the solver via:

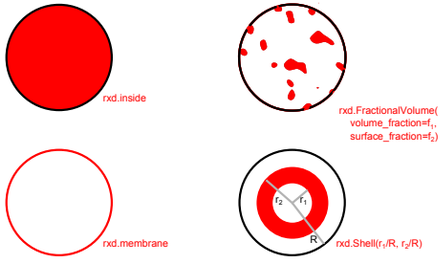
- rxd.set_solver(sol)

Model Specification

Where?



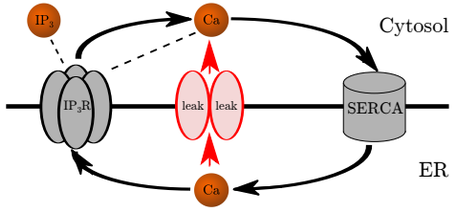
r = rxd.Region(apicals, geometry=???)



Who?

ca = rxd.Species([cyt, er],
name='ca',
charge=2)

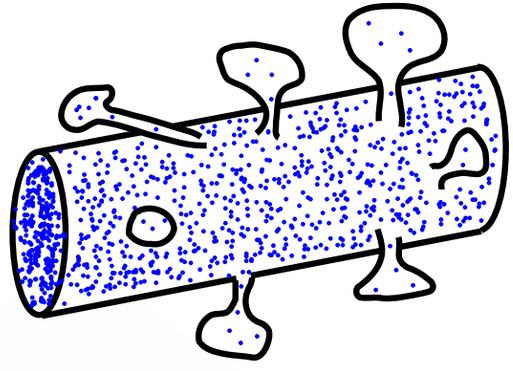
What?

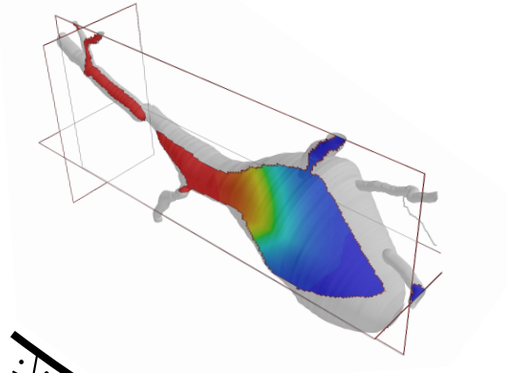


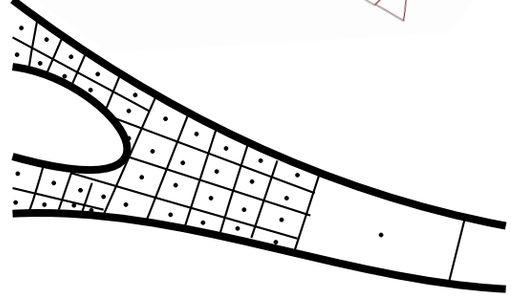
leak = rxd.MultiCompartmentReaction(
ca[er] <> ca[cyt], kf, kb,
membrane=ermem)

McDougal et al. Front Neuroinf. 2013.

Interfaces



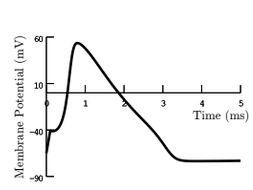


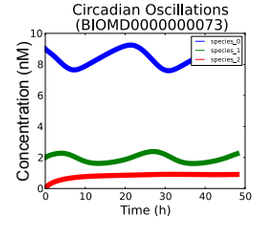


Small volumes are best modeled stochastically; changes in geometry are best modeled with a fine, high-dimensional mesh.

Difficulty: the right choice of 1D vs 3D or deterministic vs stochastic may be different for different species.

Time

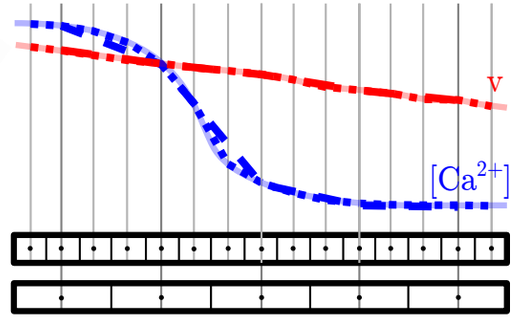




Timescales may vary wildly within the same model.

In fixed step mode, NEURON currently offers the option of only updating the reaction-diffusion on some fraction of time steps.

Space



A fine discretization helps capture changes in chemical concentrations over short distances; voltage typically takes large distances to vary significantly.

Challenges: Develop a clear and concise specification. Develop rules for branch points.

Acknowledgments

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