

Legend for Movie, CaMKII_multiburst_color.mov

This scientific visualization accompanies the manuscript entitled: “A spatial model of autophosphorylation of CaMKII in a glutamatergic spine suggests a network-driven kinetic mechanism for bistable changes in synaptic strength” posted on bioRxiv here: <https://www.biorxiv.org/content/10.1101/2024.02.02.578696v1>

The movie shows the activation of CaMKII holoenzyme within the cytoplasm of a dendritic spine, illustrated in Fig 3 of the manuscript, in response to the stimulus, shown in Fig 5 of the manuscript, between $t=0.9$ sec to $t=2.1$ sec. The onset of the stimulus begins at $t=1.0$ sec. The model shown in the movie includes all the molecules, reaction pathways, and resulting dynamics described in the manuscript but for clarity the movie visualizes only the freely diffusing Ca^{2+} ions (gold spheres), diffusing molecules of CaMKII holoenzyme (twin torus and sphere glyphs, color scheme given below), and a patch of 15 NMDARs (pentagonal receptor glyphs, color scheme given below) in the postsynaptic membrane.

Changes in the state of CaMKII holoenzyme and NMDARs are indicated by changes in color:

NMDAR

unbound:	dark green
single Glu bound:	medium green
double bound closed:	bright green
double bound open, unblocked by Mg:	white
double bound open, blocked by Mg:	red
desensitized:	dark gray

CaMKII

CaMKII is a dodecamer composed of two hexameric rings (Fig 1 of the manuscript). The six subunits of each ring can be autophosphorylated when activated. Here we represent each ring of the holoenzyme by a 2 piece glyph composed of a torus (whose color indicates the CaM-bound state of the hexameric ring) with a sphere at the center (whose color indicates the phosphorylation status of the whole ring). The holoenzyme is represented by two of these torus-with-sphere assemblies stacked back-to-back. The color scheme is:

Torus representing a single hexameric ring:

0 CaM4 bound:	red
1 CaM4 bound:	green
2 CaM4 bound:	blue
3 CaM4 bound:	cyan
4 CaM4 bound:	magenta
5 CaM4 bound:	yellow
6 CaM4 bound:	white

Sphere representing the phosphorylation status of a single hexameric ring:

0 subunits phosphorylated:	black
1 subunits phosphorylated:	red
2 subunits phosphorylated:	green
3 subunits phosphorylated:	blue
4 subunits phosphorylated:	cyan
5 subunits phosphorylated:	magenta
6 subunits phosphorylated:	yellow

