ManyLands: A Journey Across 4D Phase Space of Trajectories

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USE CASES

In this document, we provide the mathematical descriptions of the dynamical systems that were used during the use cases, together with the initial conditions and the integration duration that were employed in the ODE solver (outside of *ManyLands*). We provide also screenshots that were retrieved during the use cases by the domain scientists. These correspond to the figures that were used in the paper. A detailed analysis of each case has been already provided by the domain scientists, and is documented in the paper.

1) USE CASE (A) - Analysis of the Bipolar Disorder Model

ODEs:

```
eps = 0.01
dx = (0.16 / (0.16 + y  * y)) * ((2 * z) / (1 + 2 * z)) - x /
(1 + 2 * x)
dy = (0.16 / (0.16 + x * x)) * ((2 * w) / (1 + 2 * w)) - y /
(1 + 2 * y)
dw = eps * (y - z)
dz = eps * (x - w)
```

Initial Conditions:

```
x0 = 0.0, y0 = 0.0, w0 = 1.8, z0 = 0.0
```

Duration:

```
t = [0, 6000], timestep = 1
```

Screenshots retrieved during the session with the domain scientists. A detailed visual analysis of the system with the use of our tool has been provided in Use Case (A) of the paper.

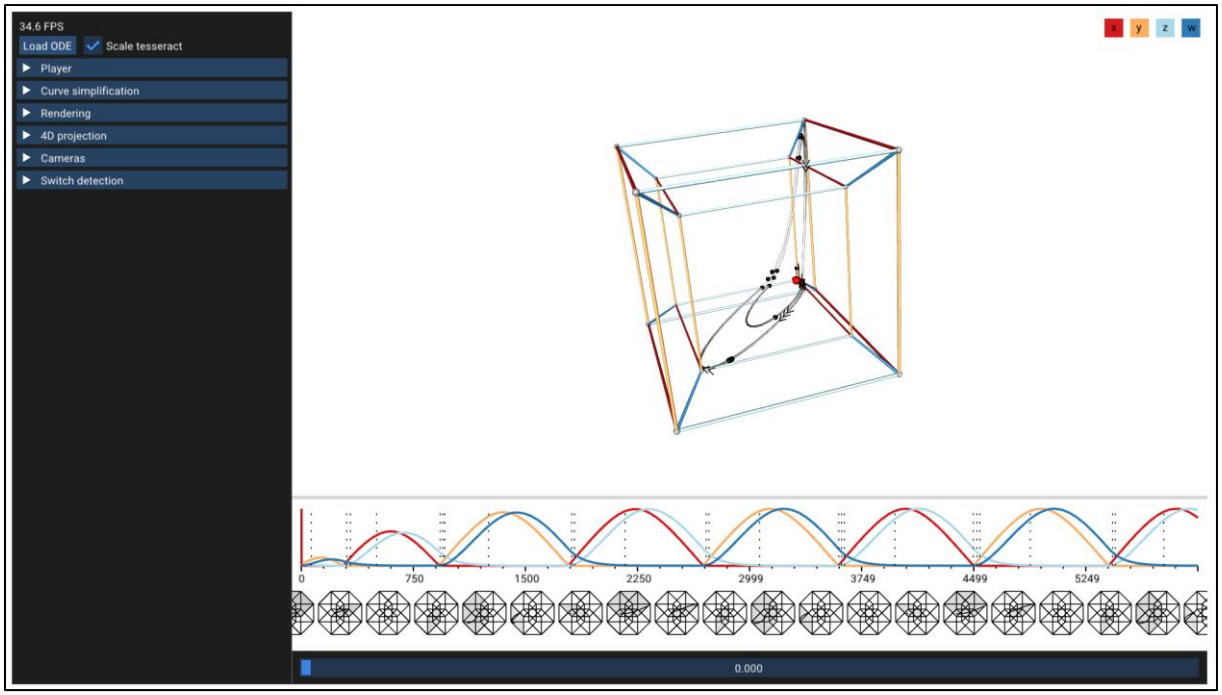

Figure: 4D HyperLand of the Bipolar Disorder Model

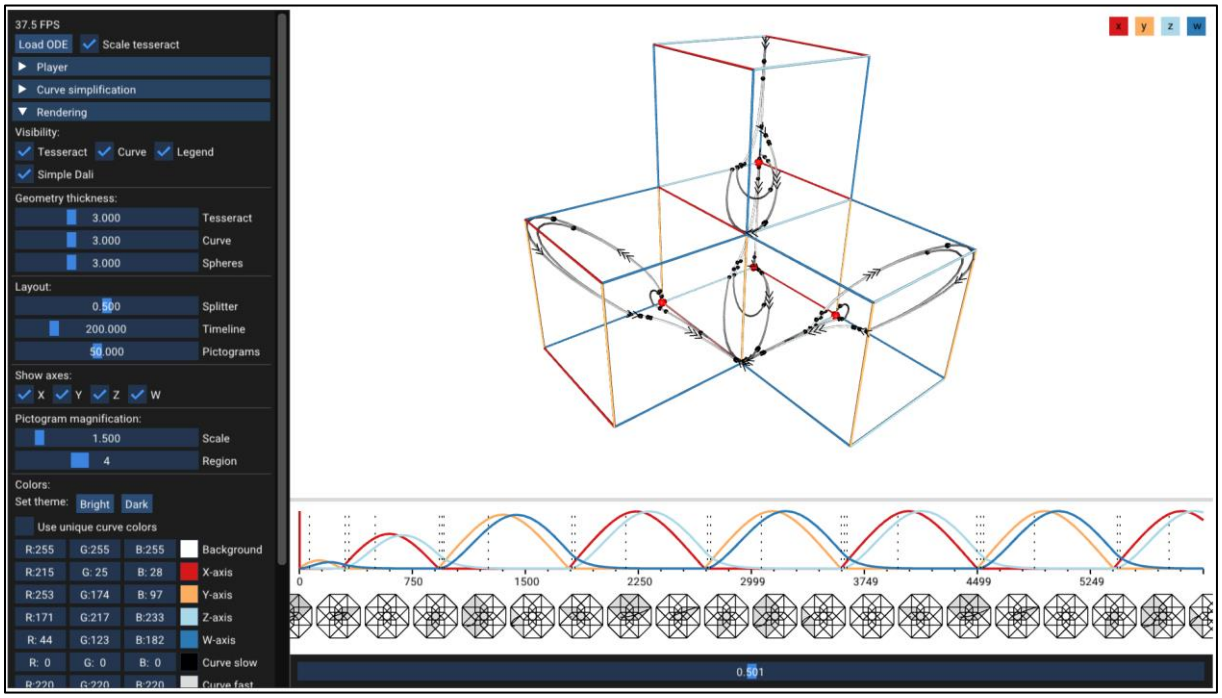

Figure: 3D reduced SpaceLand of the Bipolar Disorder Model

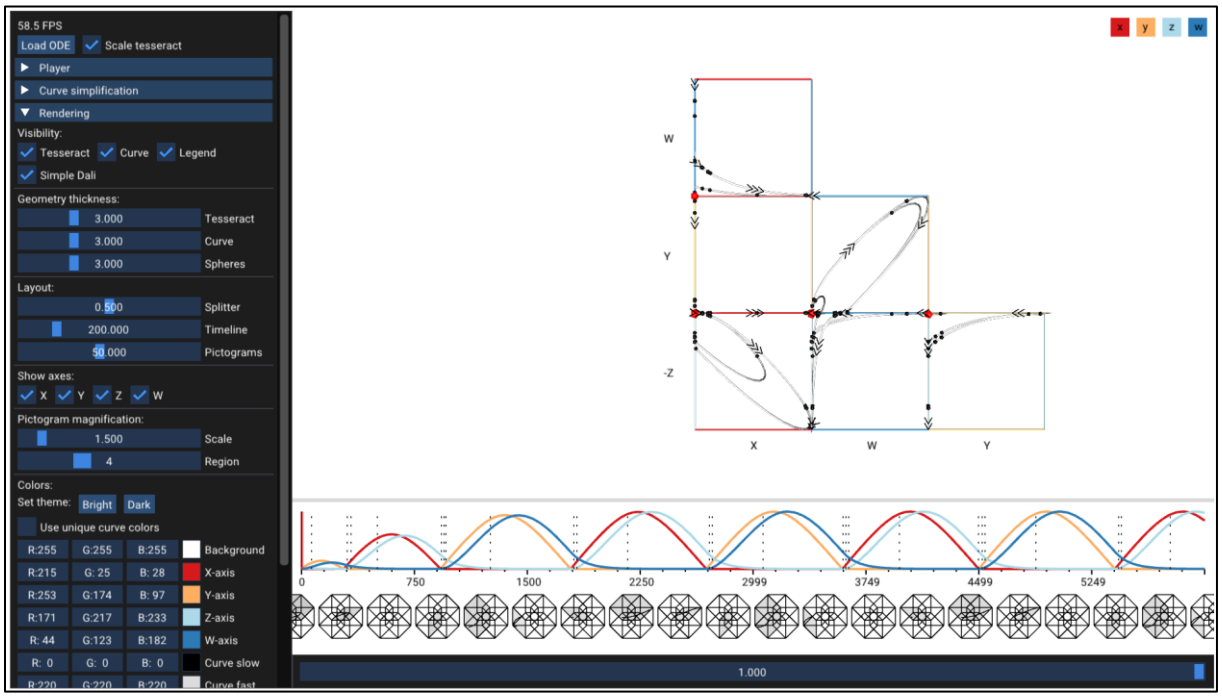

Figure: 2D FlatLand of the Bipolar Disorder Model

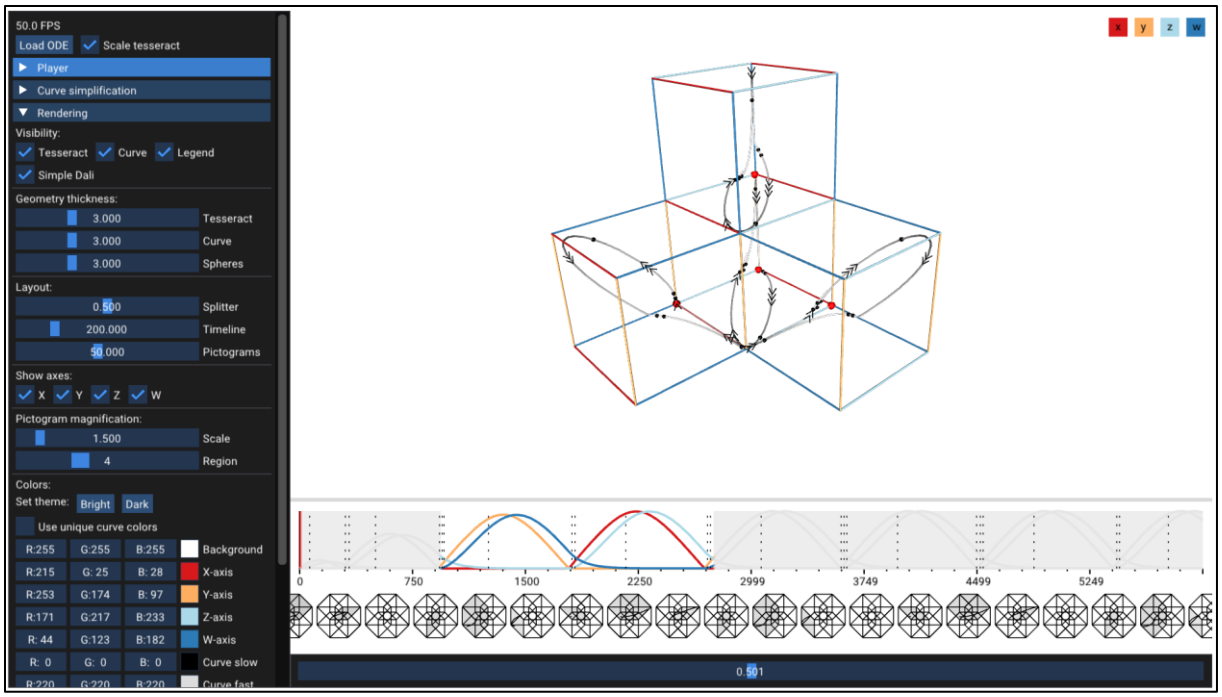

Figure: 3D reduced SpaceLand of the Bipolar Disorder Model (repetitive closed trajectory)

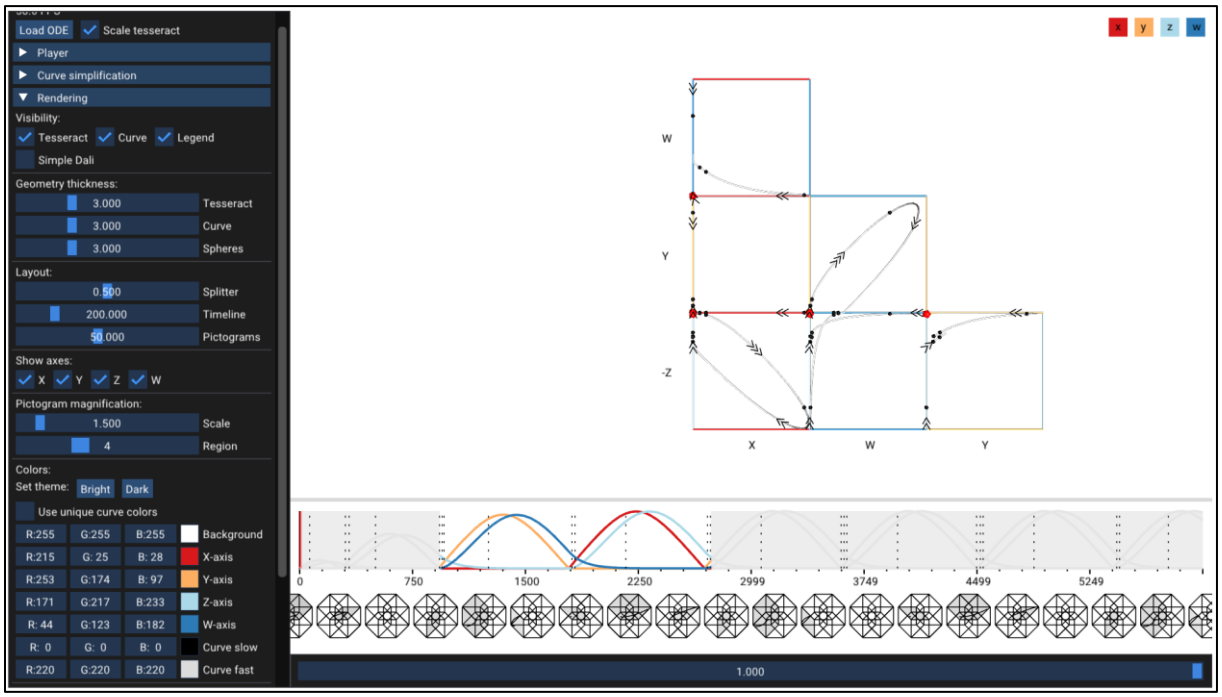

Figure: 2D FlatLand of the Bipolar Disorder Model (repetitive closed trajectory)

2) USE CASE (B) - Analysis of the NF-κB Pathway

ODEs:

```
kNin = 5.4
kIin = 0.018
kIout = 0.012
kNIout = 0.83
kt = 1.03
kt1 = 0.24
kf = 30
kfn = 30
kb = 0.03
kbn = 0.03
alpha = 1.05 * 0.5
gamma = 0.017
k3 = 0.00001
k1 = 0.00001
dx = kNin * k3 * (1 - x) / (k3 + z) - kNIout * w * x / (k1 + x)
dy = kt * x * x * x - gamma * y
dz = kt1 * y - alpha * (1 - x) * z / (k3 + z) - kIin * z +
kIout * w * k1 / (k1 + x)
dw = kIin * z - kIout * w * k1 / (k1 + x) - kNIout * w * x /
(k1 + x)
```

Initial Conditions:

```
1) x0 = 0.4, y0 = 6.0, z0 = 0.0, w0 = 5.0
2) x0 = 0.0, y0 = 6.0, z0 = 0.0, w0 = 5.0
```

Duration:

```
t = [0, 1000], timestep = 0.1
```

Screenshots retrieved during the session with the domain scientists. A detailed visual analysis of the system with the use of our tool has been provided in Use Case (B) of the paper.

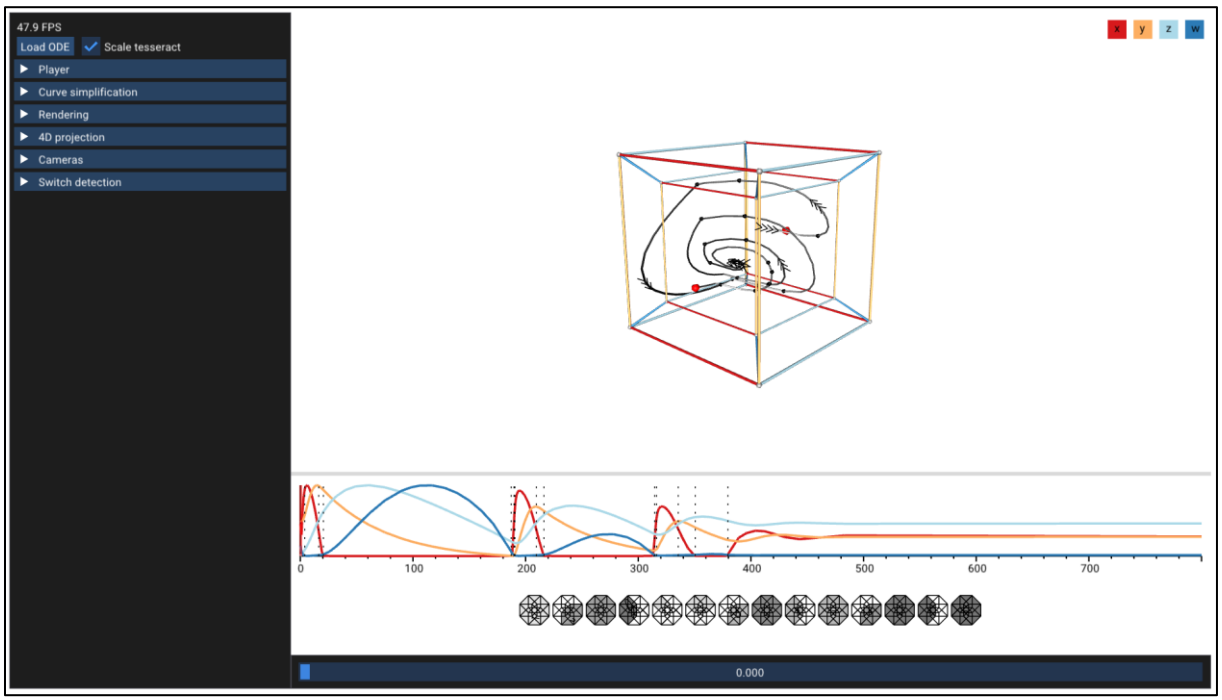

Figure: 4D HyperLand of the NF-κB Model (with two solutions)

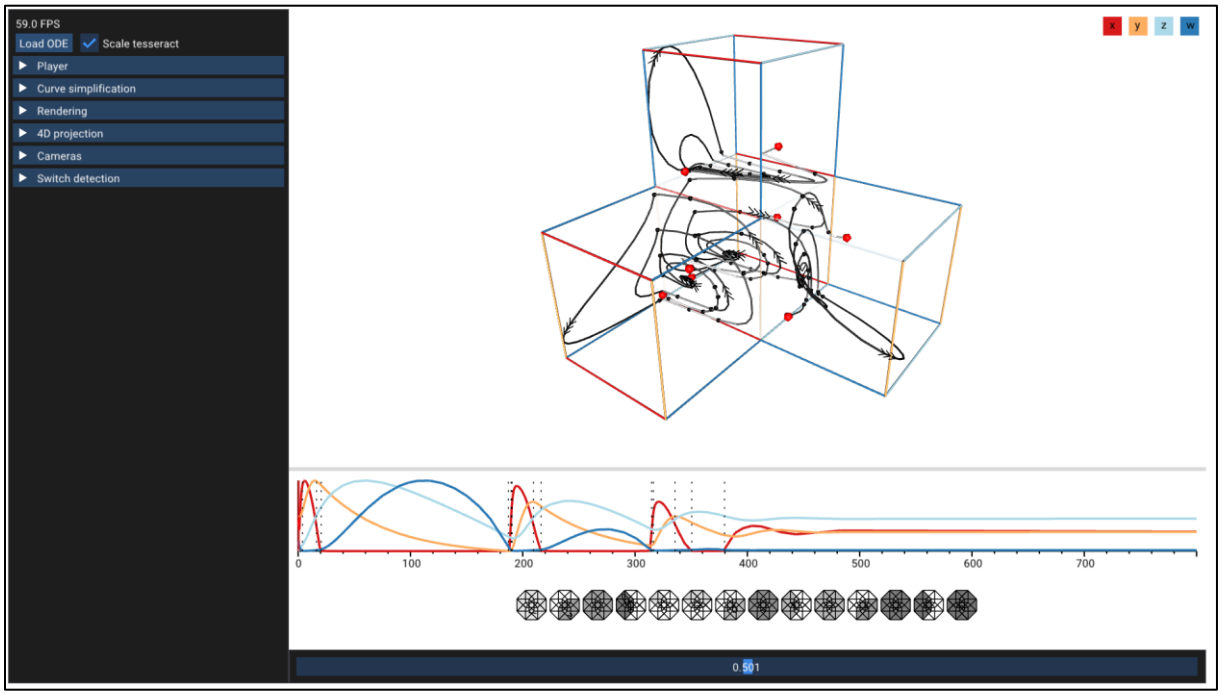

Figure: 3D reduced SpaceLand of the NF-κB Model (with two solutions)

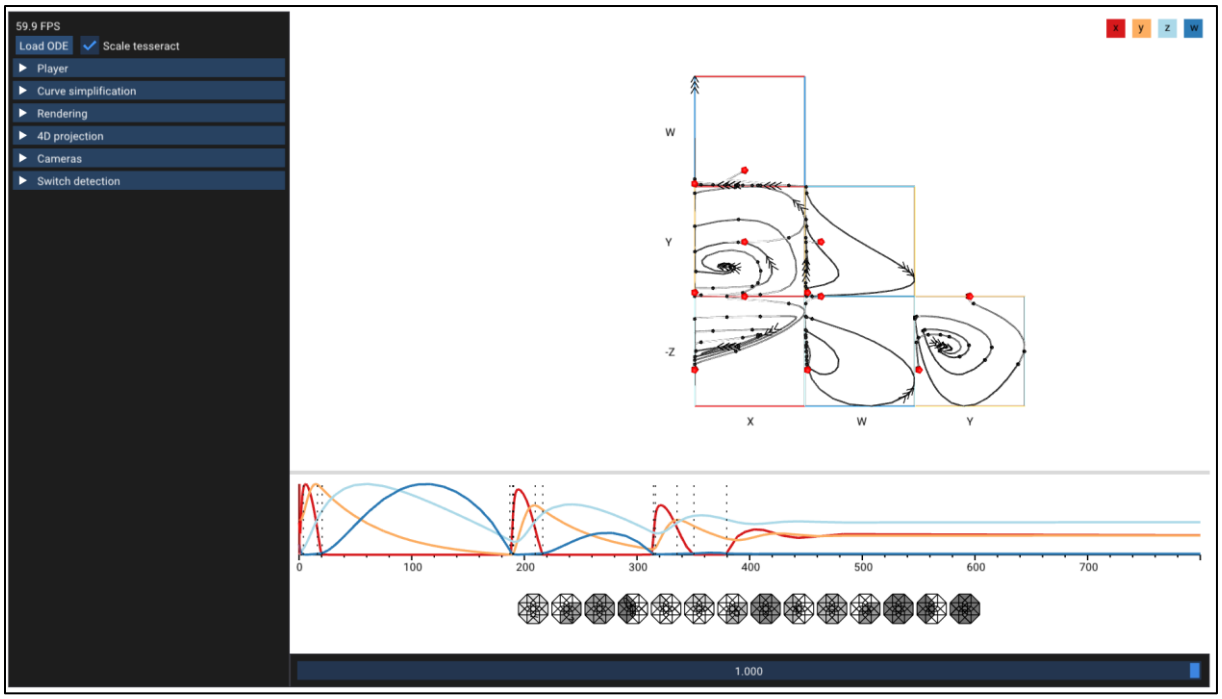

Figure: 2D FlatLand of the NF-κB Model (with two solutions)

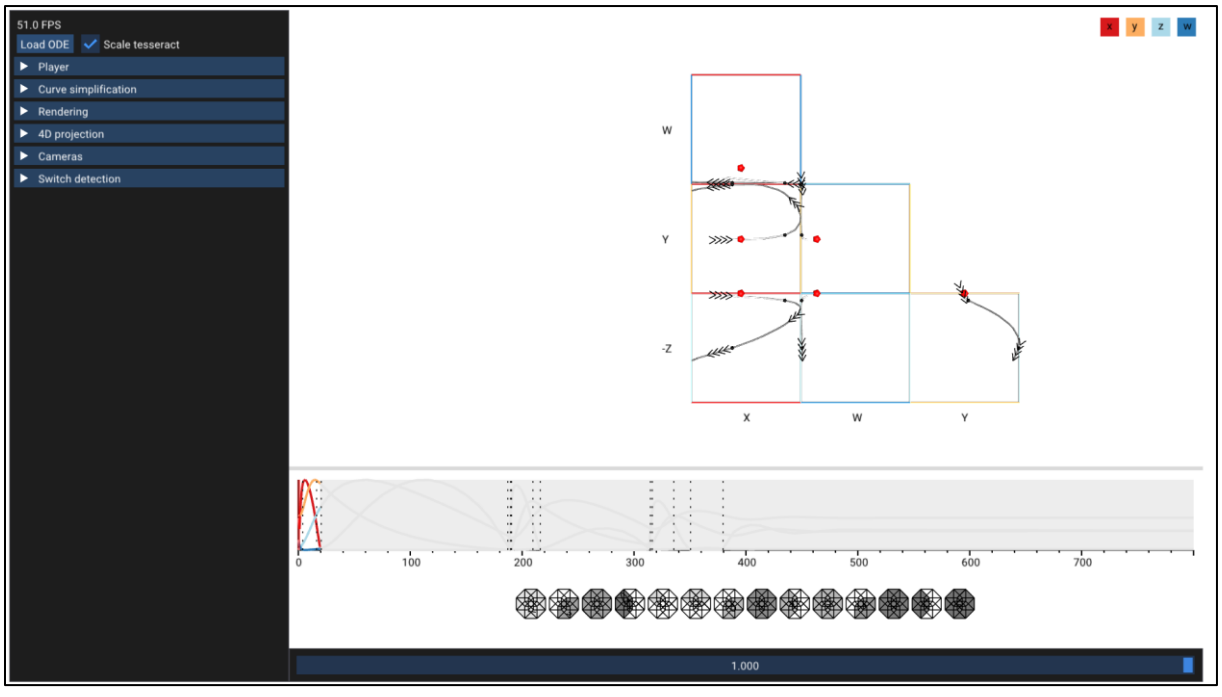

Figure: 2D FlatLand of the NF-κB Model (selection of fast behavior)

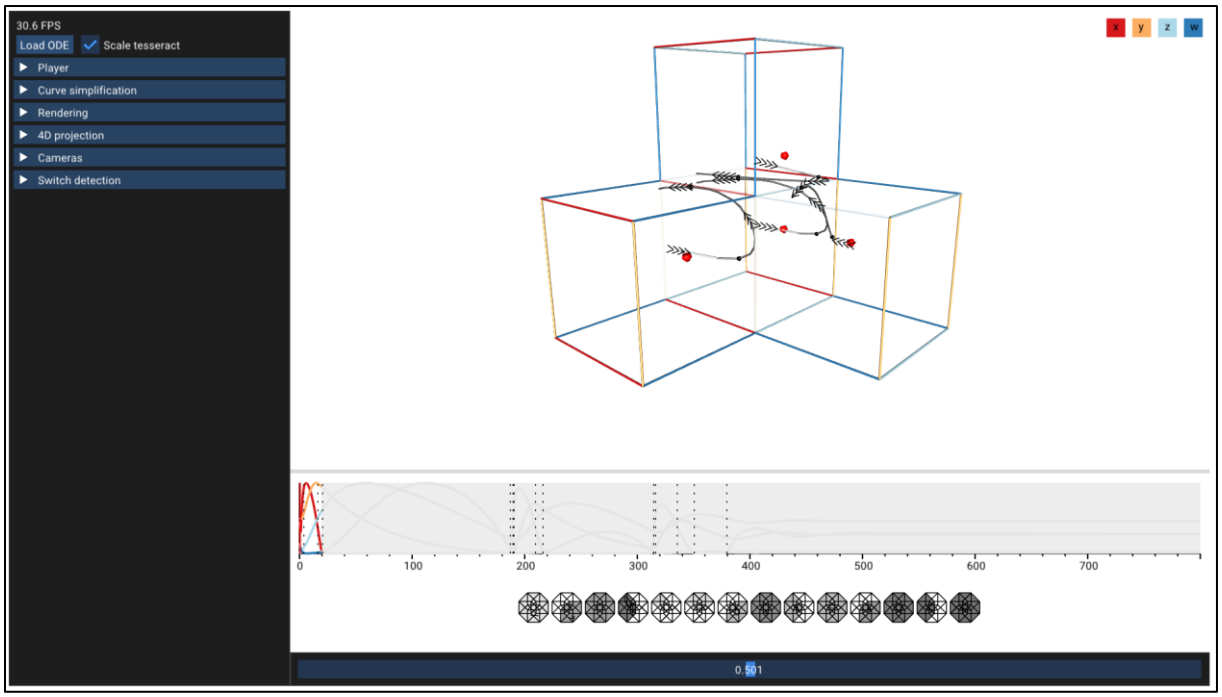

Figure: 3D reduced SpaceLand of the NF-κB Model (selection of fast behavior)

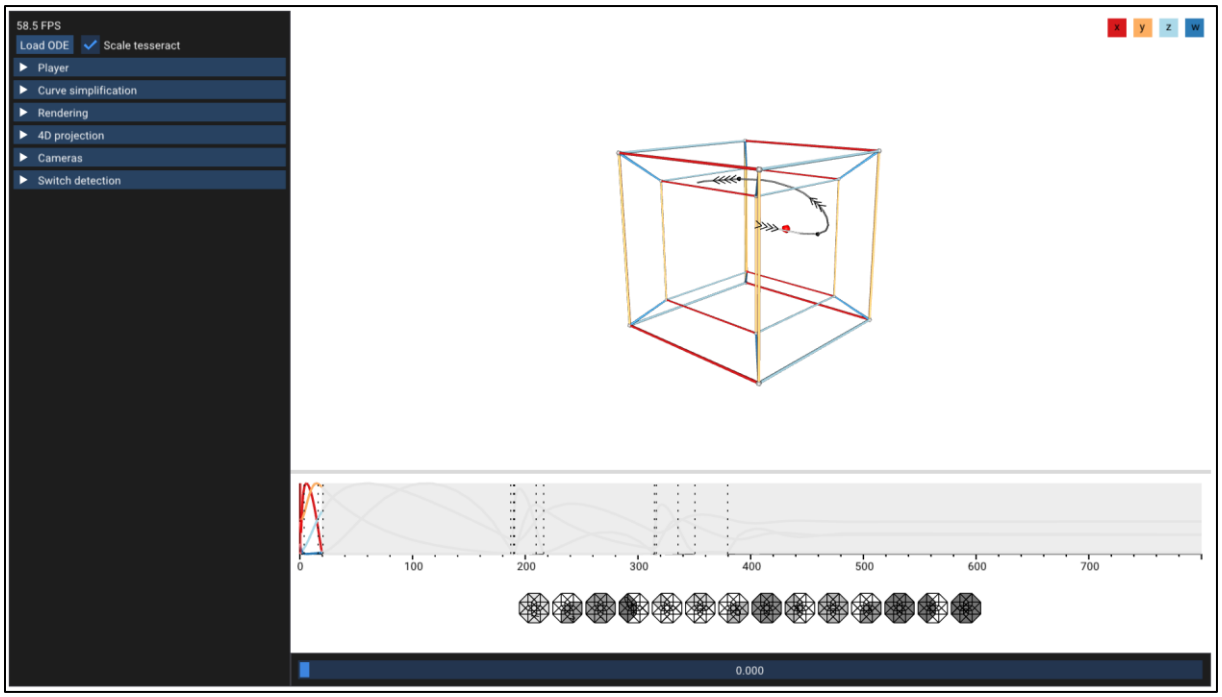

Figure: 4D HyperLand of the NF-κB Model (selection of fast behavior)

3) USE CASE (C) - Analysis of Peroxidase-Oxidase Reaction with Olsen Model

ODEs:

```
k1 = 0.35
k2 = 250
k3 = 0.035
k4 = 20
k5 = 5.35
k6 = 0.0001
k7 = 0.8
k_7 = 0.1
k8 = 0.825

dA = -k3 * A * B * Y + k7 - k_7 * A
dB = -k3 * A * B * Y - k1 * B * X + k8
dX = k1 * B * X - 2 * k2 * X * X + 3 * k3 * A * B * Y - k4 * X + k6
dY = -k3 * A * B * Y + 2 * k2 * X * X - k5 * Y
```

Initial Conditions:

```
A0 = 0.0, B0 = 0.0, X0 = 0.0, Y0 = 0.0
```

Duration:

```
t = [0, 300], timestep = 0.07
```

Screenshots retrieved during the session with the domain scientists. A detailed visual analysis of the system with the use of our tool has been provided in Use Case (C) of the paper.

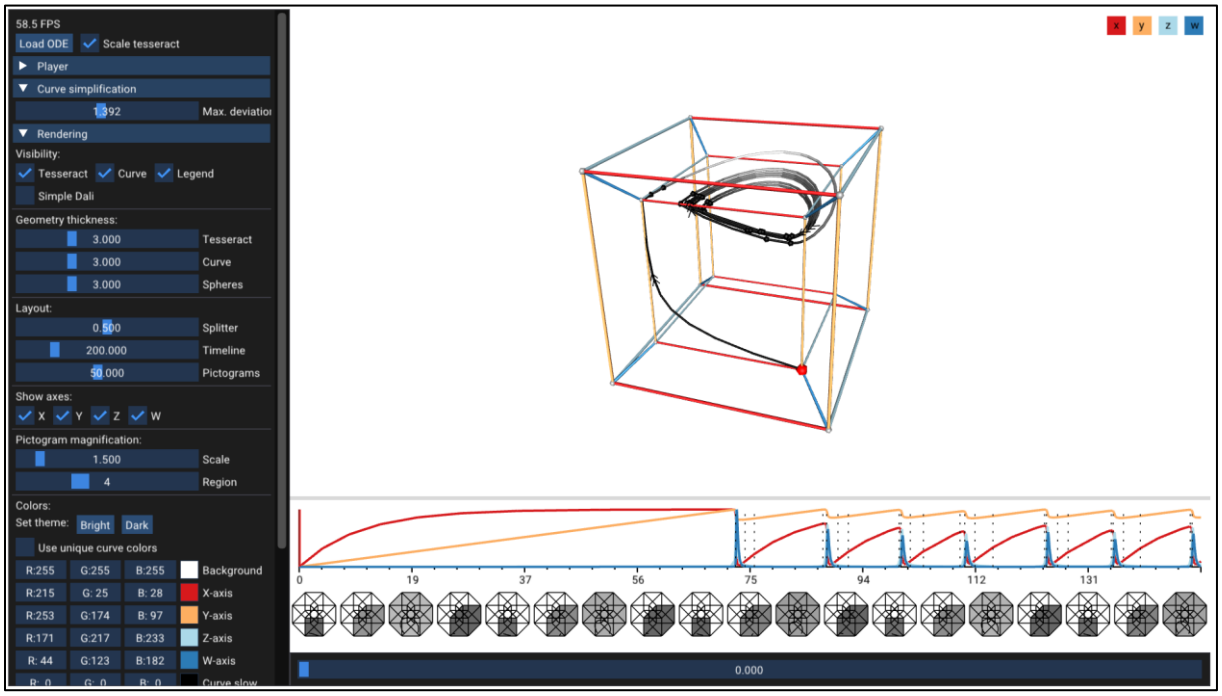

Figure: 4D HyperLand of the Olsen Model

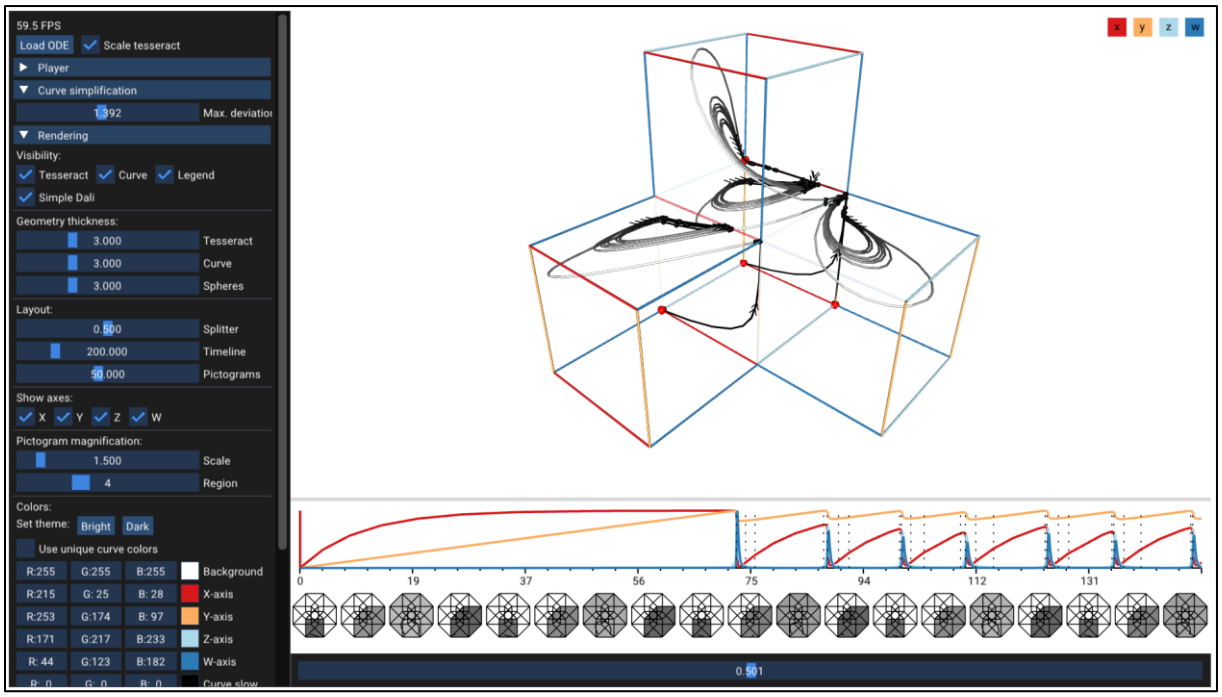

Figure: 3D reduced SpaceLand of the Olsen Model

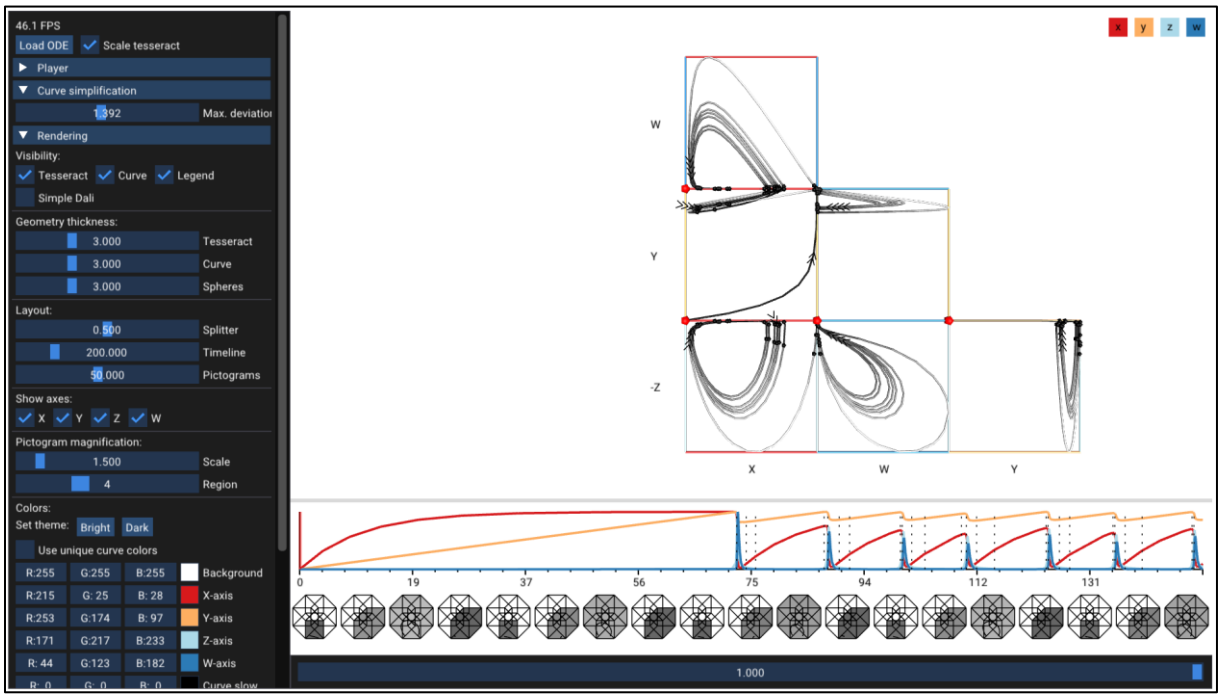

Figure: 2D FlatLand of the Olsen Model

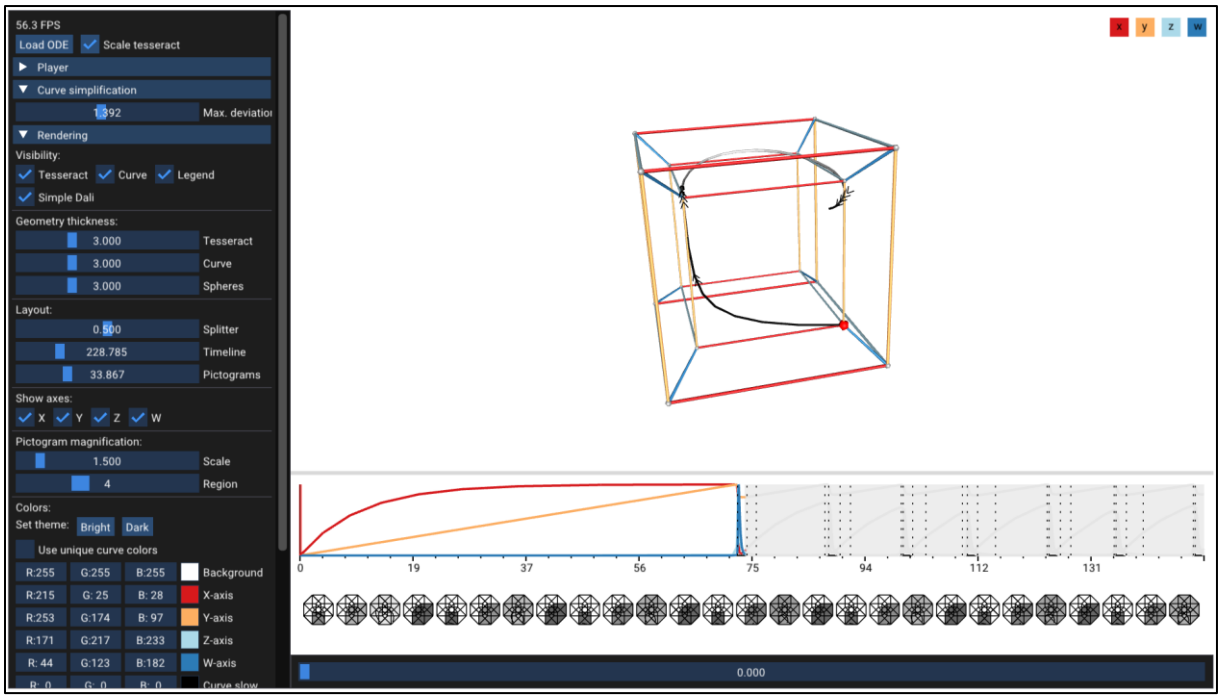

Figure: 4D HyperLand of the Olsen Model (selection of the fast behavior)

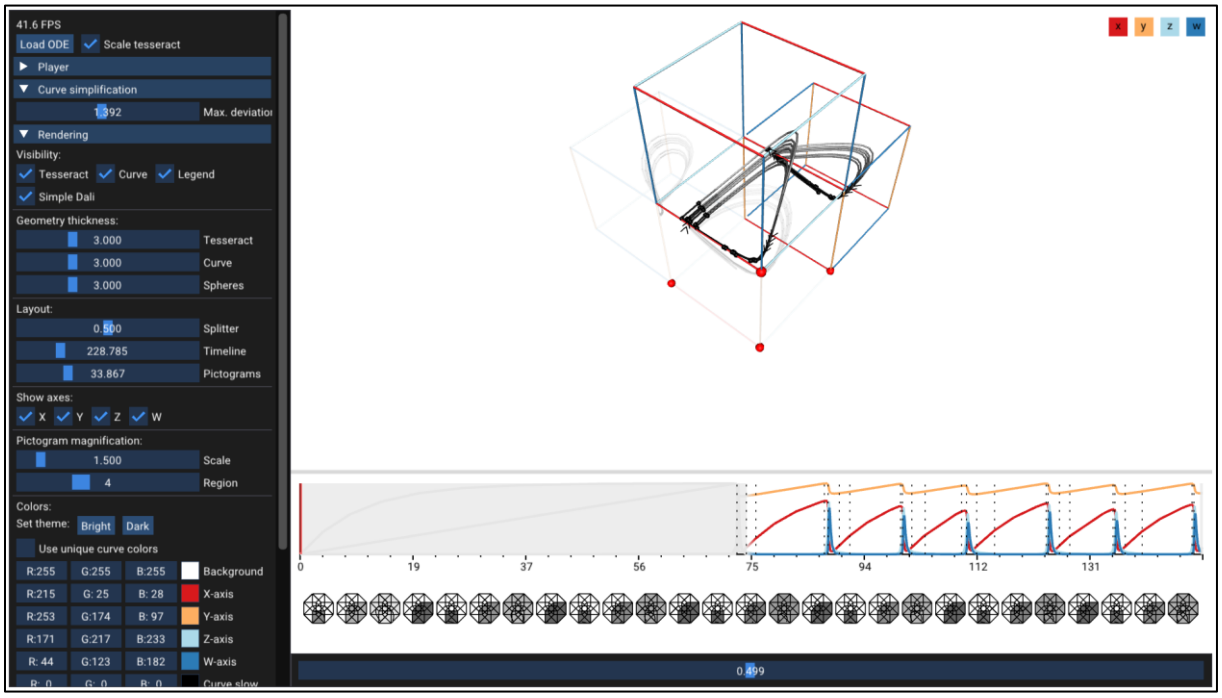

Figure: 3D reduced SpaceLand of the Olsen Model (selection of the periodic oscillation)

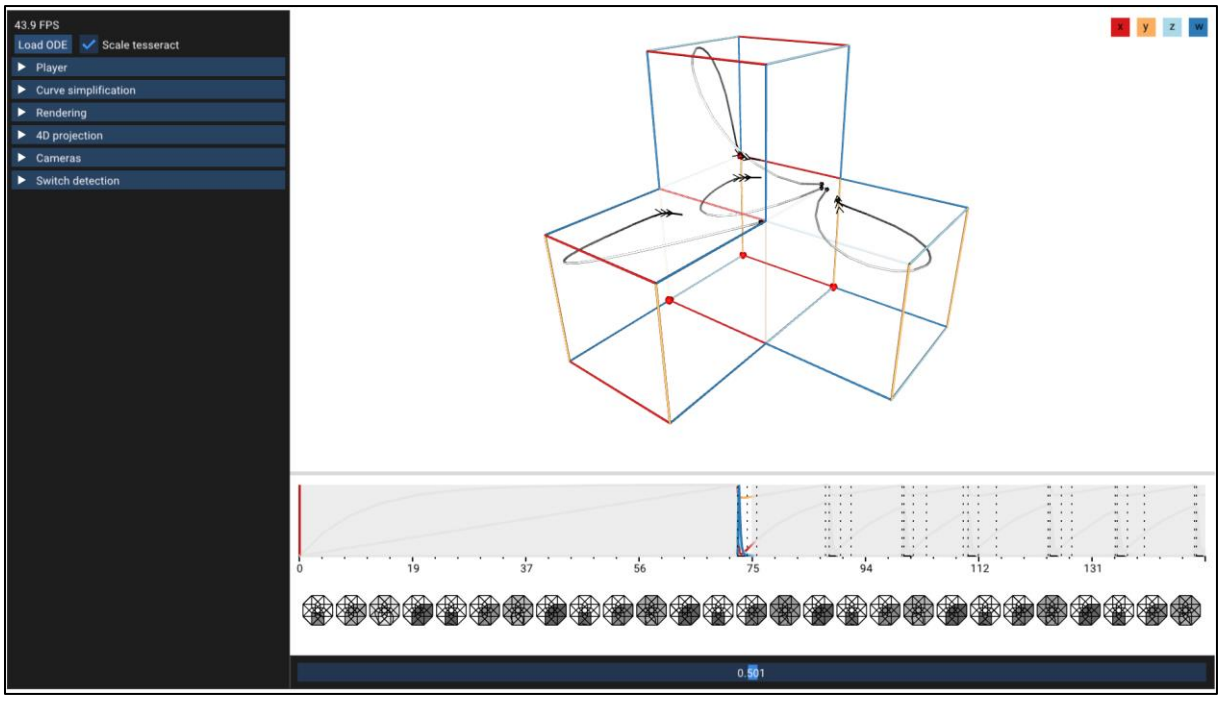

Figure: 3D reduced SpaceLand of the Olsen Model (selection of the switch between behaviors)