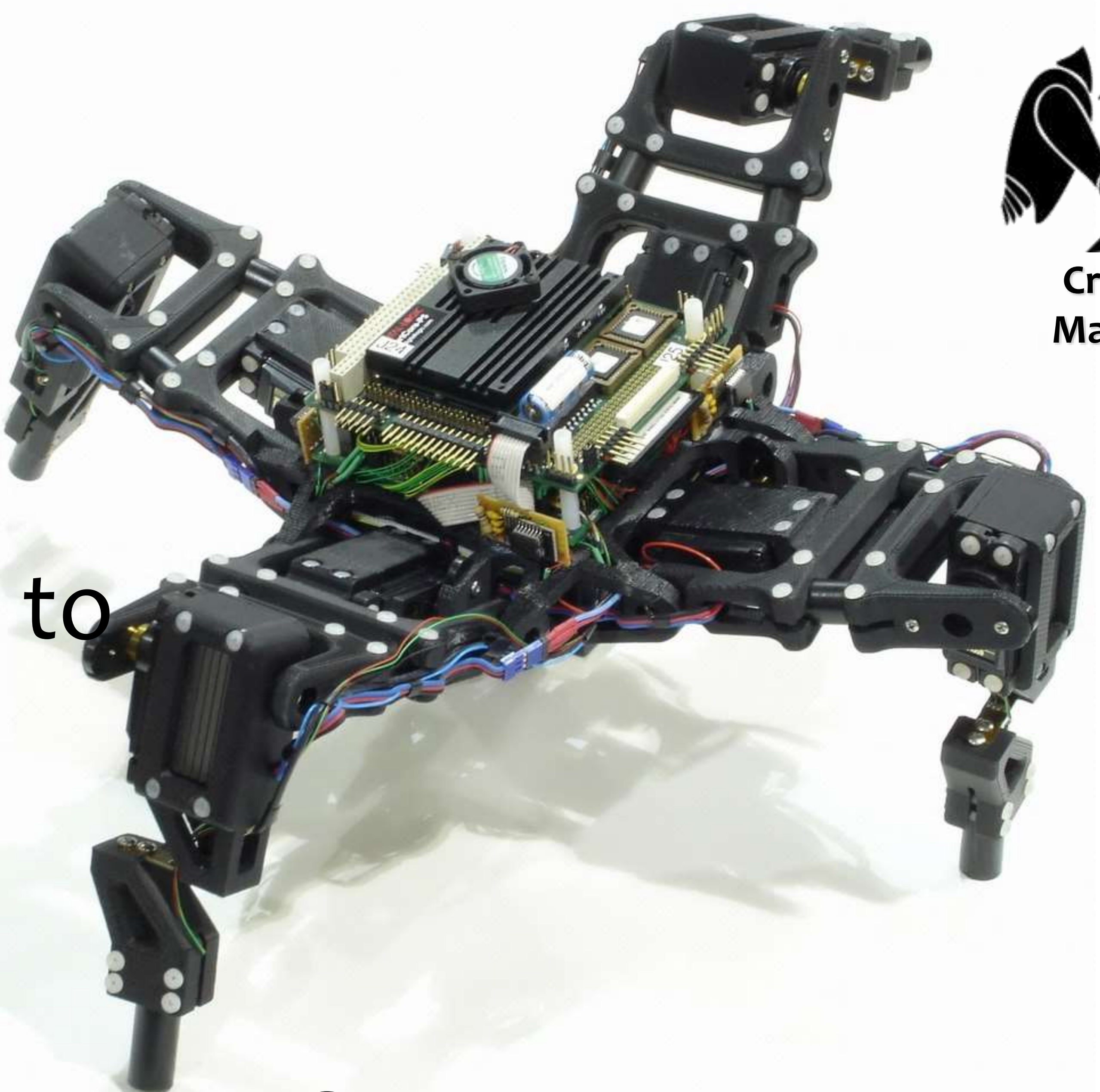
The AI Scientist

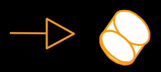
Automating discovery, from cognitive robotics to computational biology



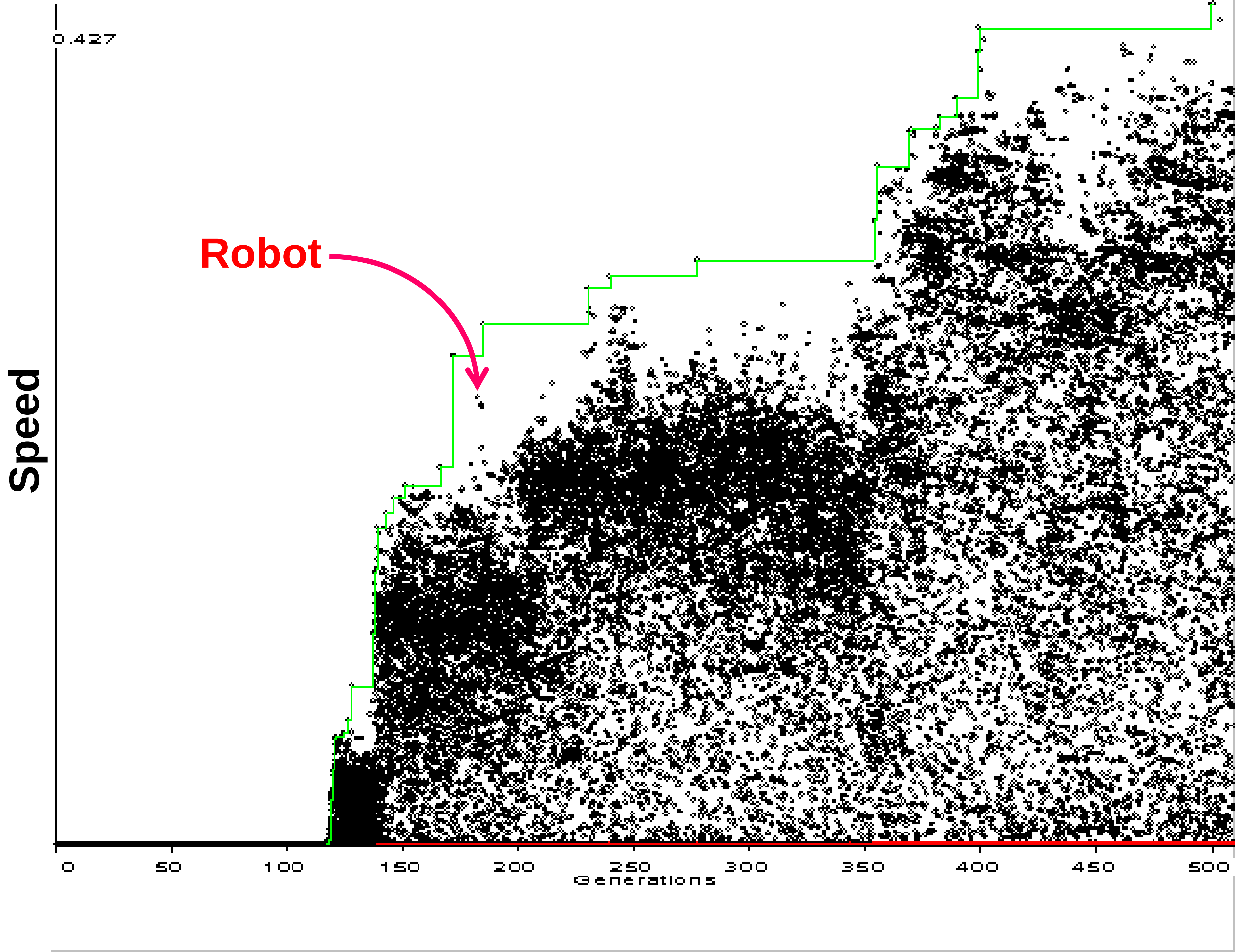
Creative Machines Lab

For copy of slides email **Hod.Lipson@Columbia.edu**

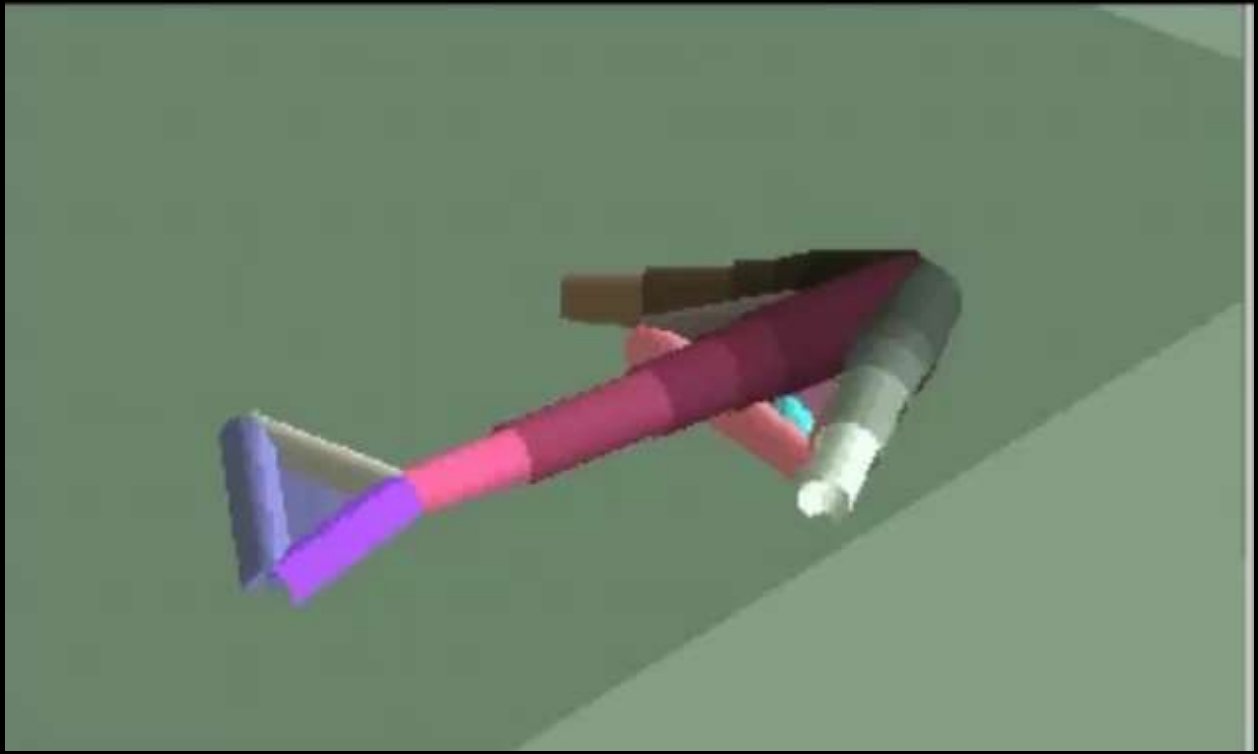
Evolution



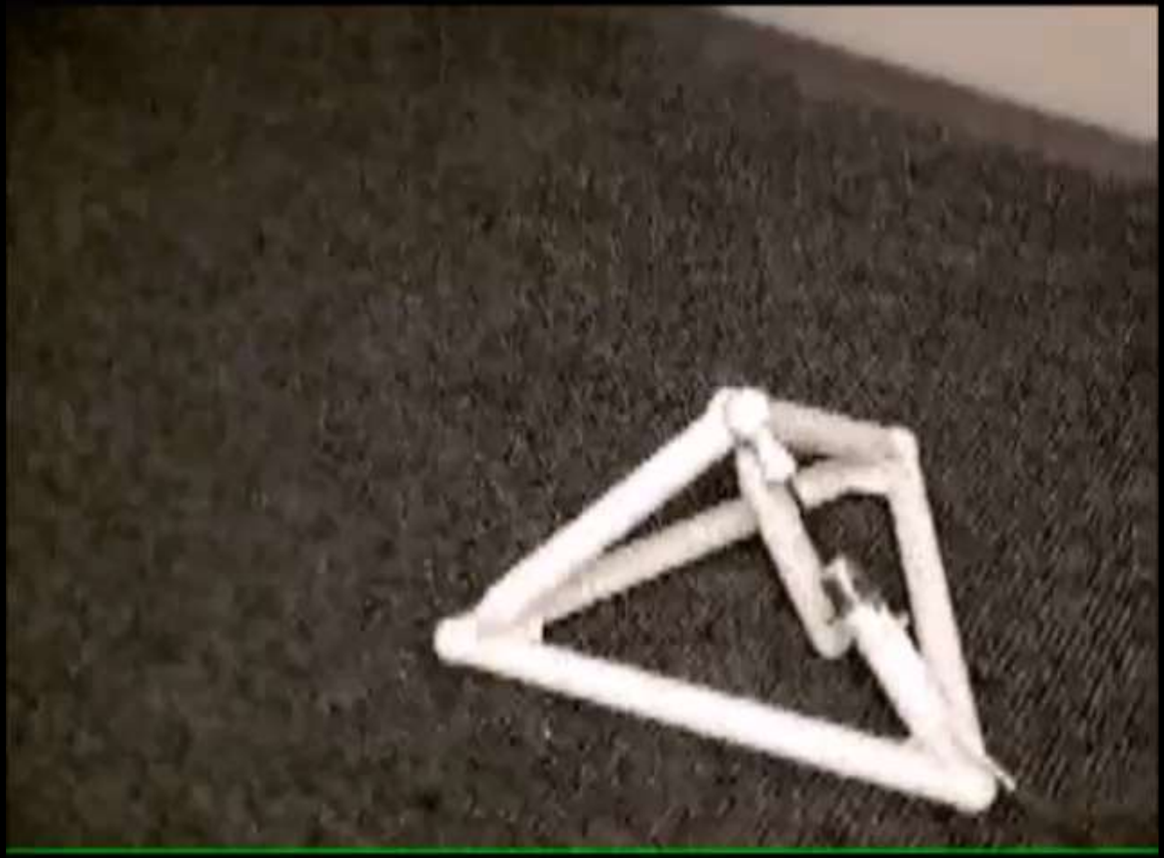

SiliconGraphics
Computer Systems
ONYX



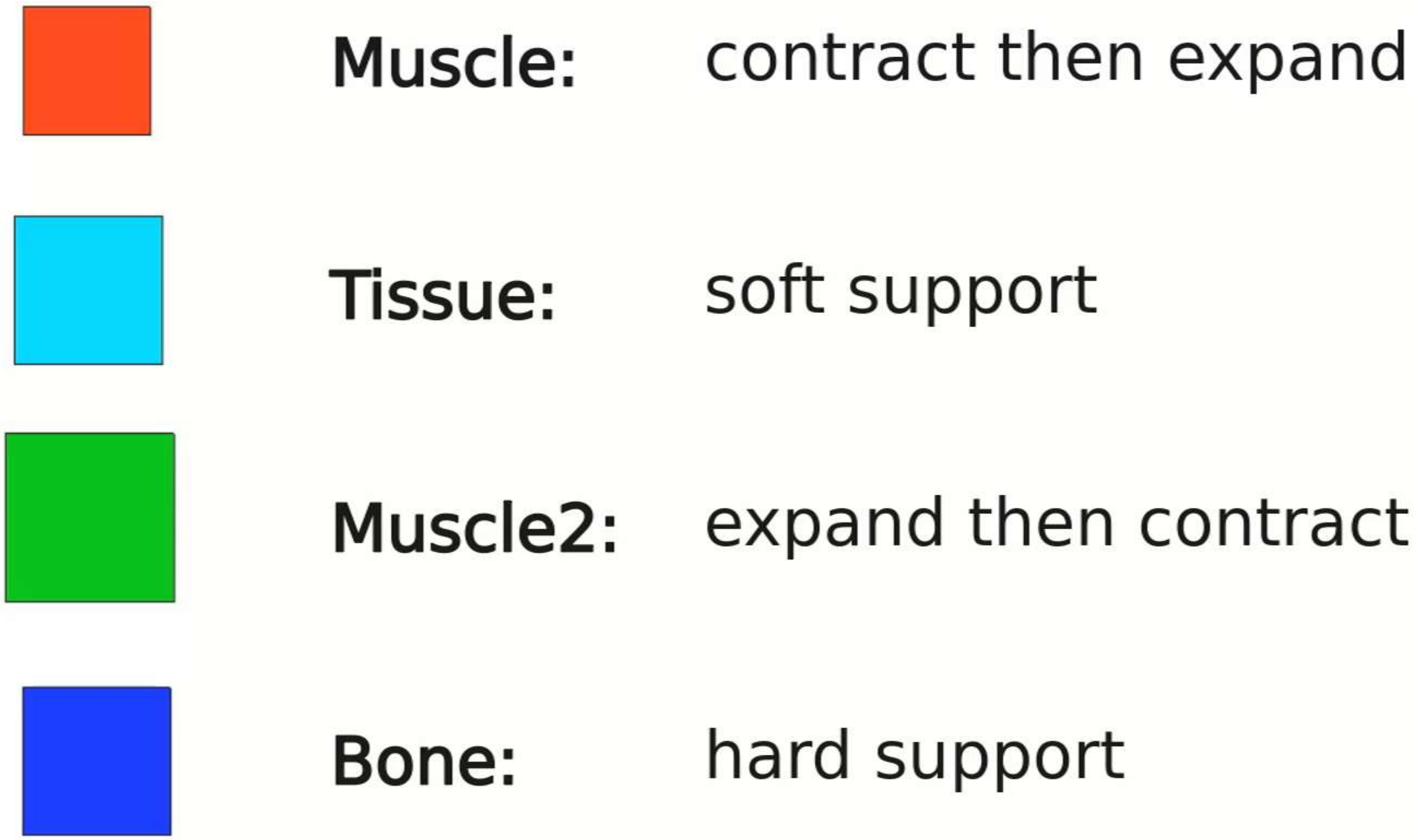
0.427
Robot
Speed
0
50
100
150
200
250
300
350
400
450
500
Generations



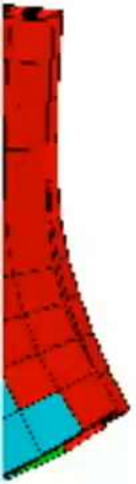
Lipson & Pollack, Nature 406, 2000



Lipson & Pollack, Nature 406, 2000



With Nick Cheney



Miriyev et al, (2017) *Nature Communications*

The New York Times

THURSDAY, AUGUST 31, 2000

Scientists Report They Have Made Robot That Makes Its Own Robots

By KENNETH CHANG

For the first time, computer scientists have created a robot that designs and builds other robots, almost entirely without human help.

In the short run, this advance could lead to a new industry of inexpensive robots customized for specific tasks. In the long run — decades at least — robots may one day be truly regarded as "artificial life," able to reproduce and evolve, building improved versions of themselves.

Such durable, adaptive robots, astronomers have suggested, could someday be sent into space to explore the galaxy or search for other life.

But the quest to create artificial

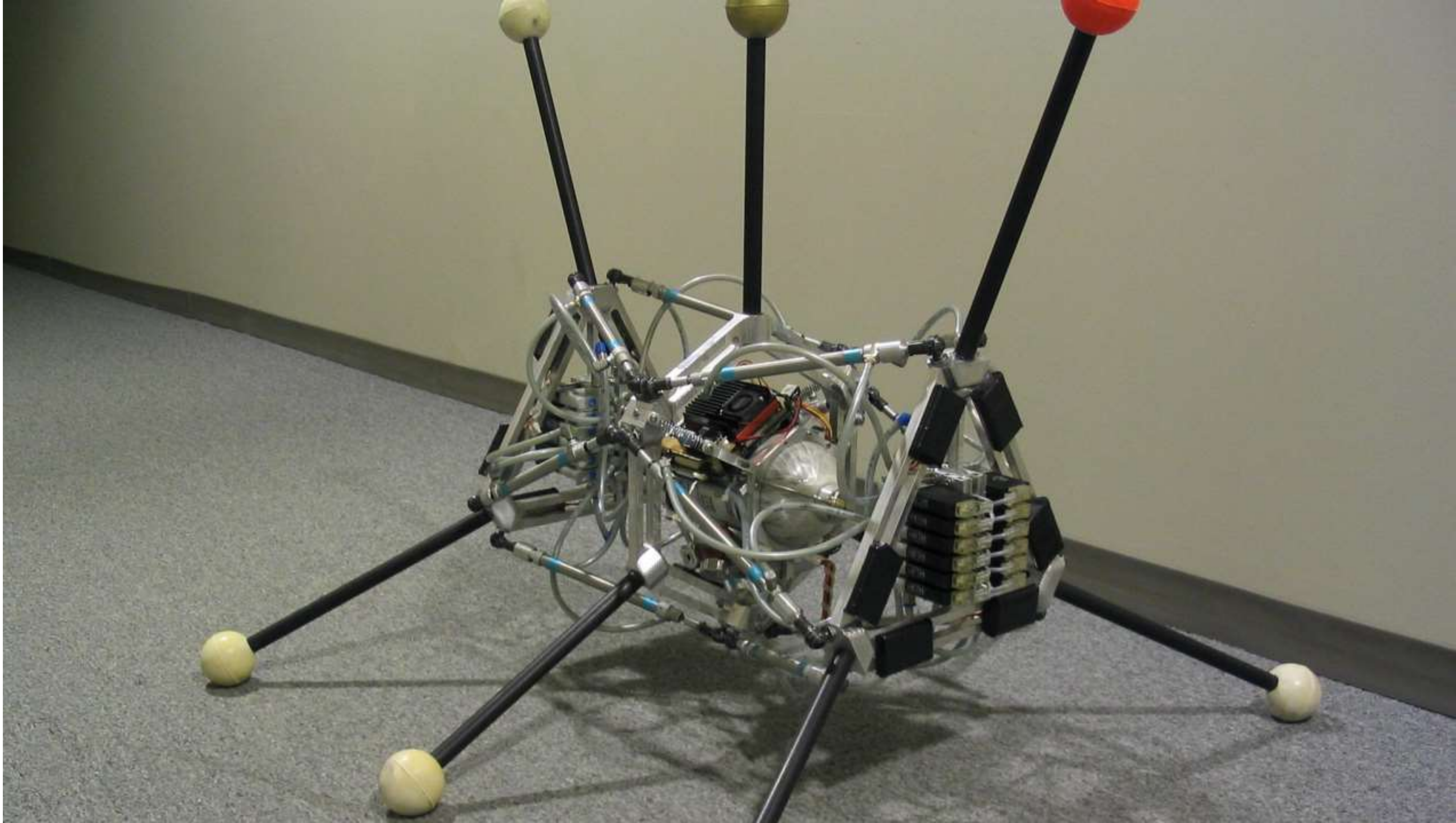
Brandeis University

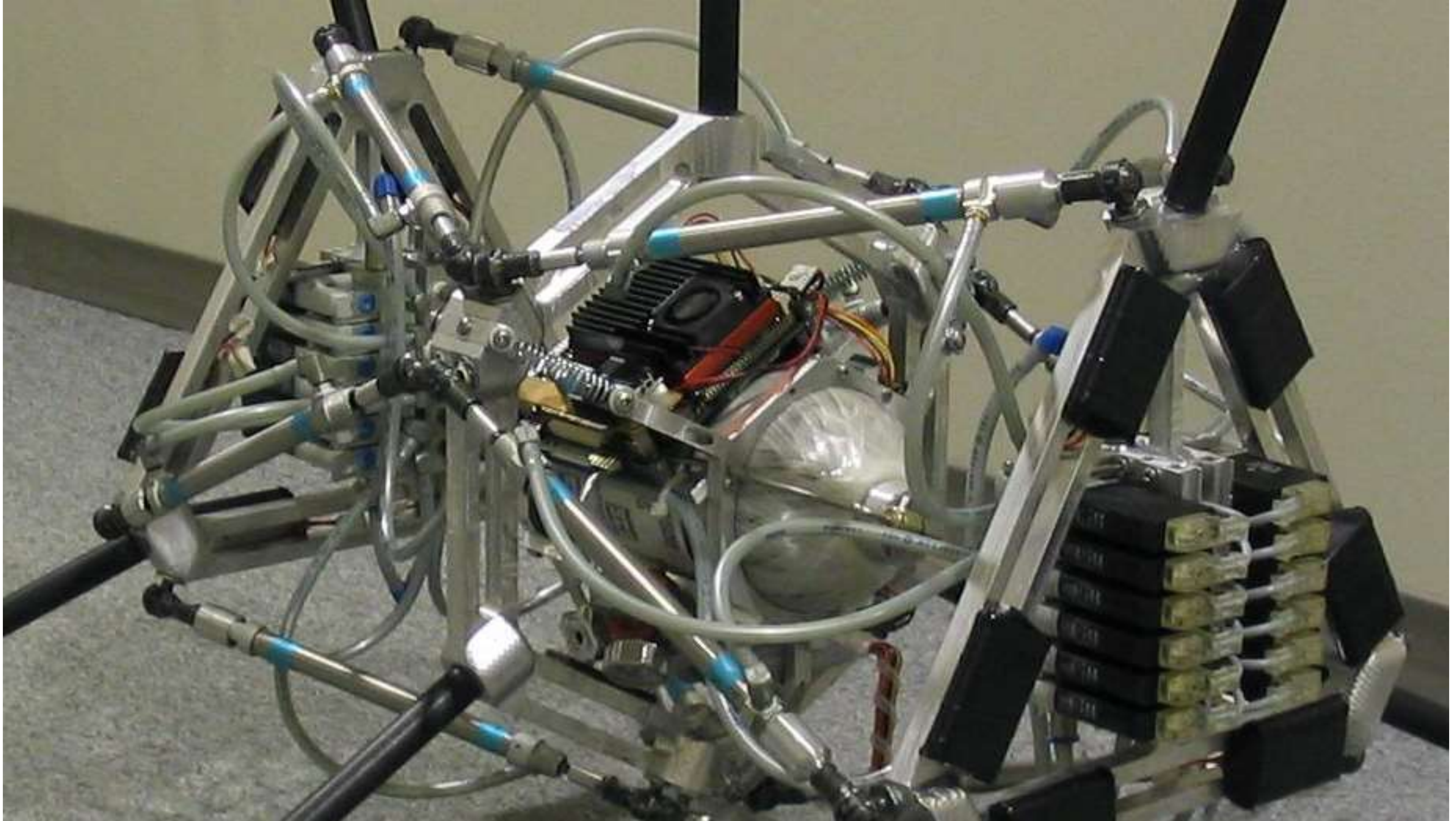
The "Arrow" left a trail as it crawled across a bed of sand.

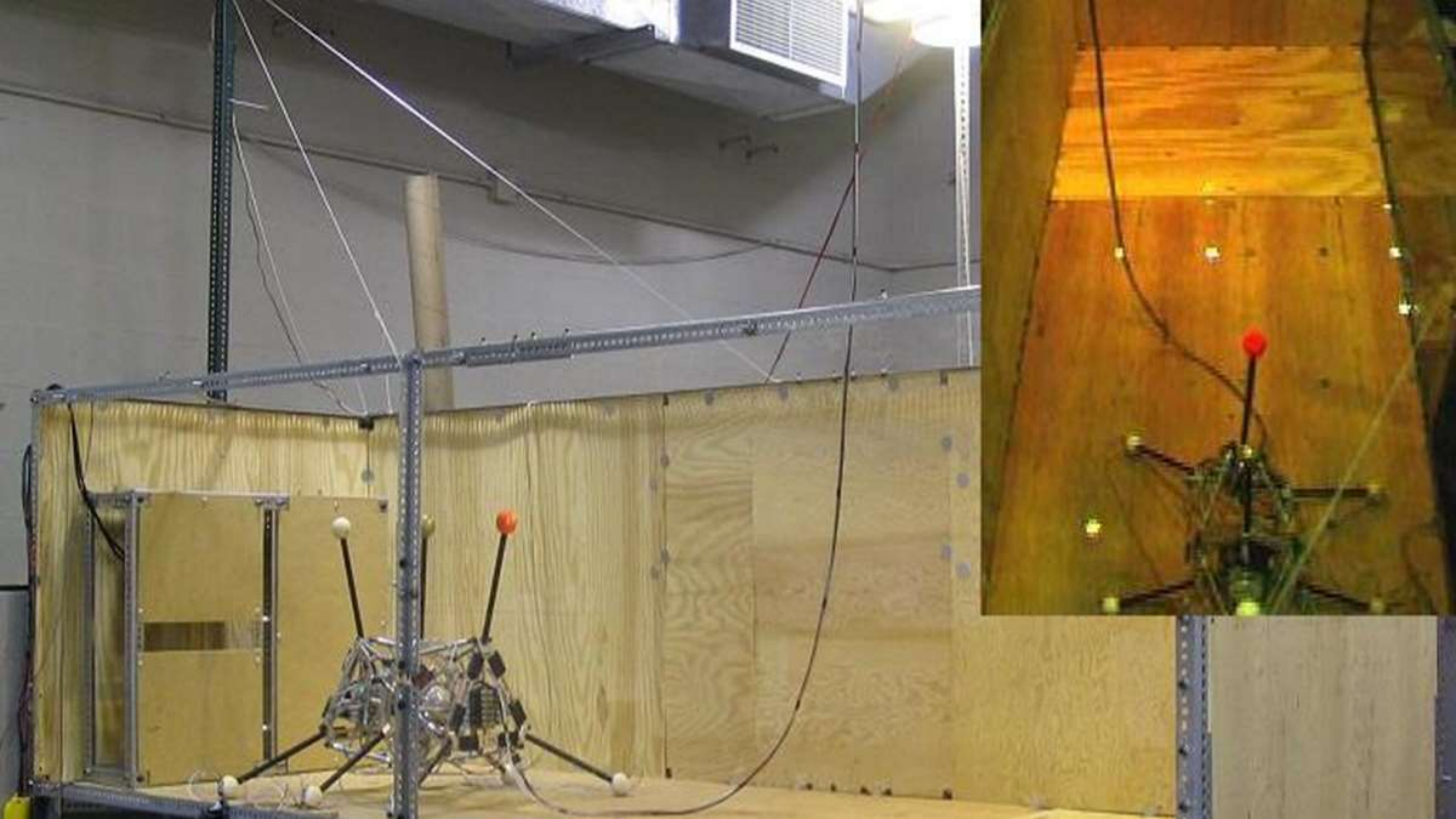
were not manufactured by humans."

Dr. Pollack and Dr. Lipson, a research scientist, report their results in today's issue of the journal Nature.

"This is the first example of

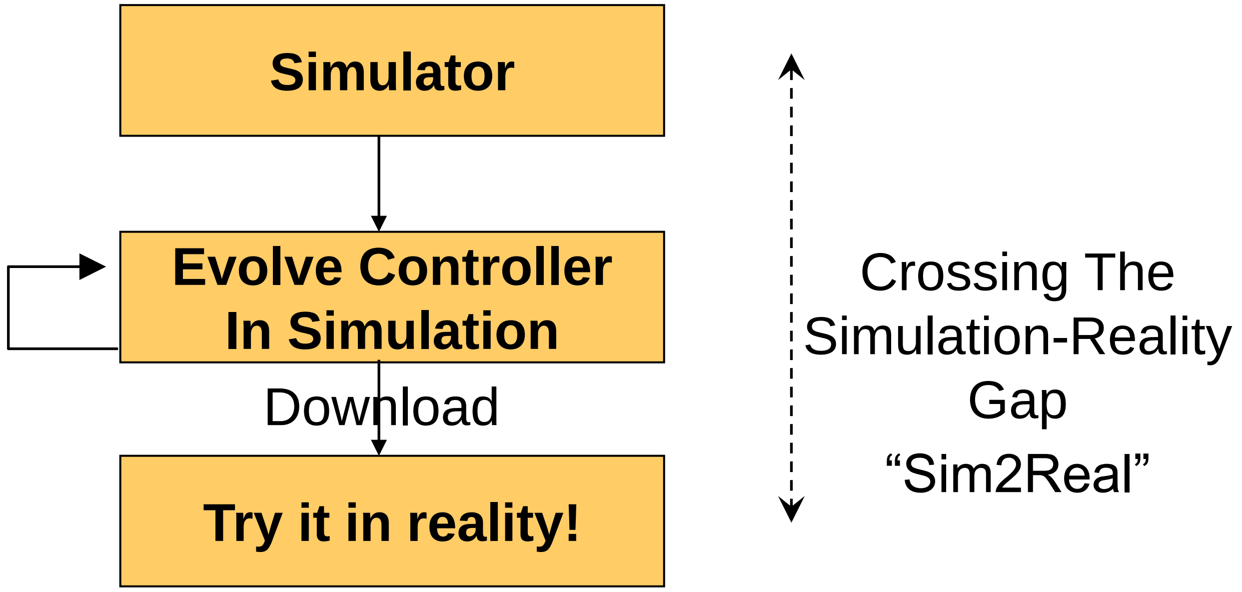




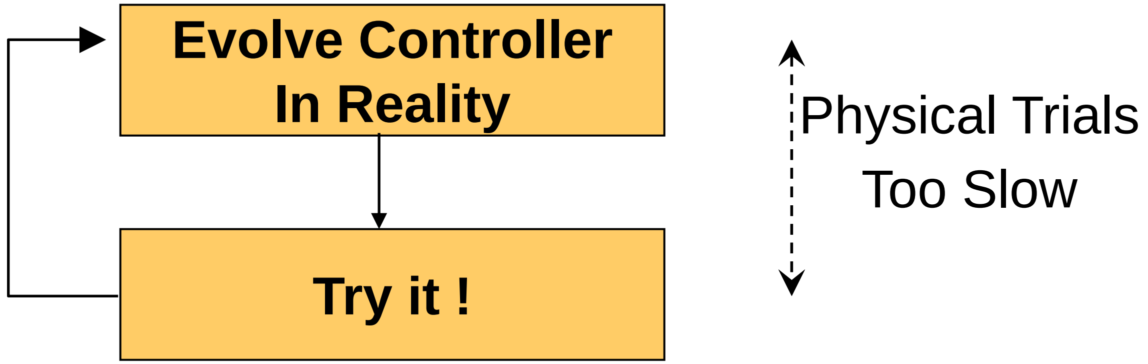


With Viktor Zykov and Josh Bongard

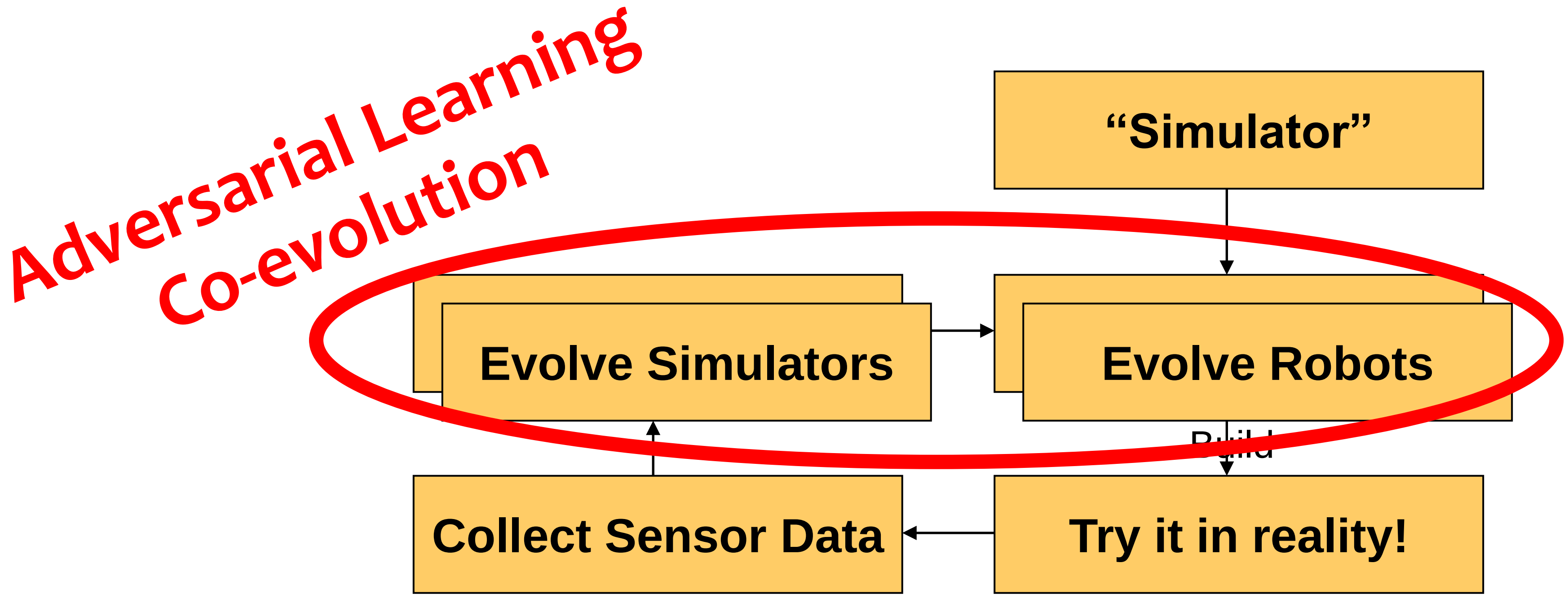
Adapting in simulation

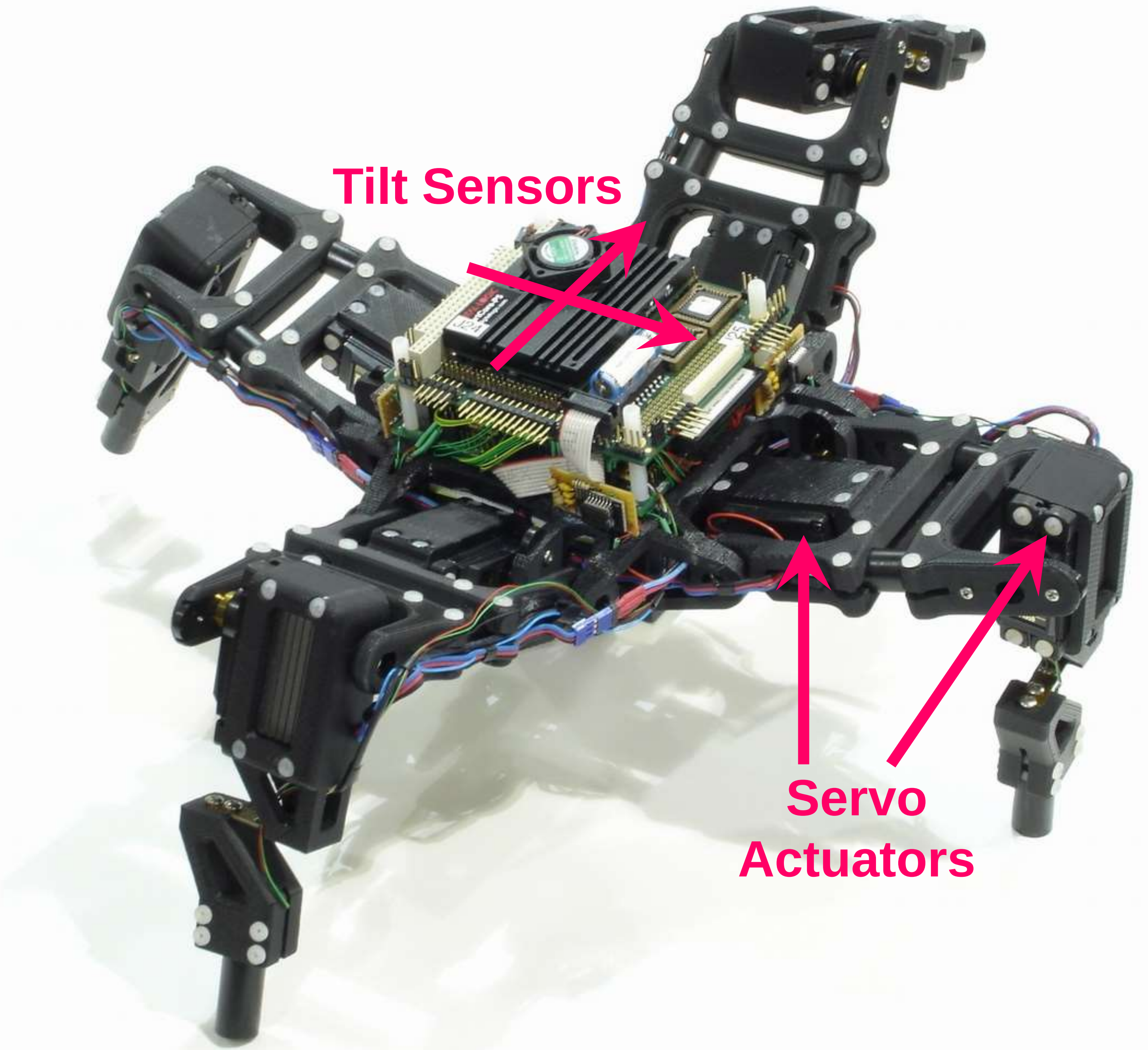


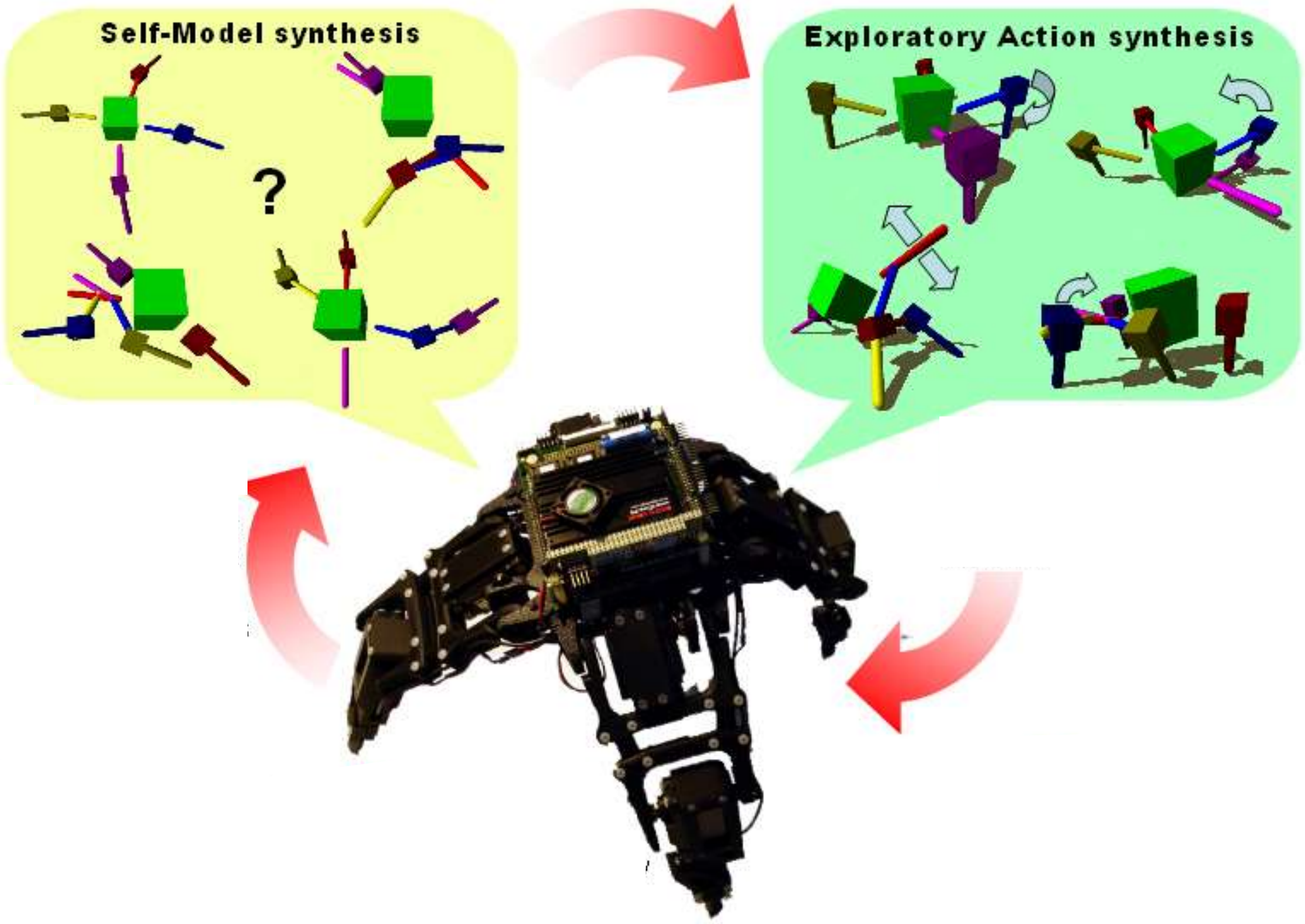
Adapting in reality



Simulation & Reality




Tilt Sensors
Servo
Actuators

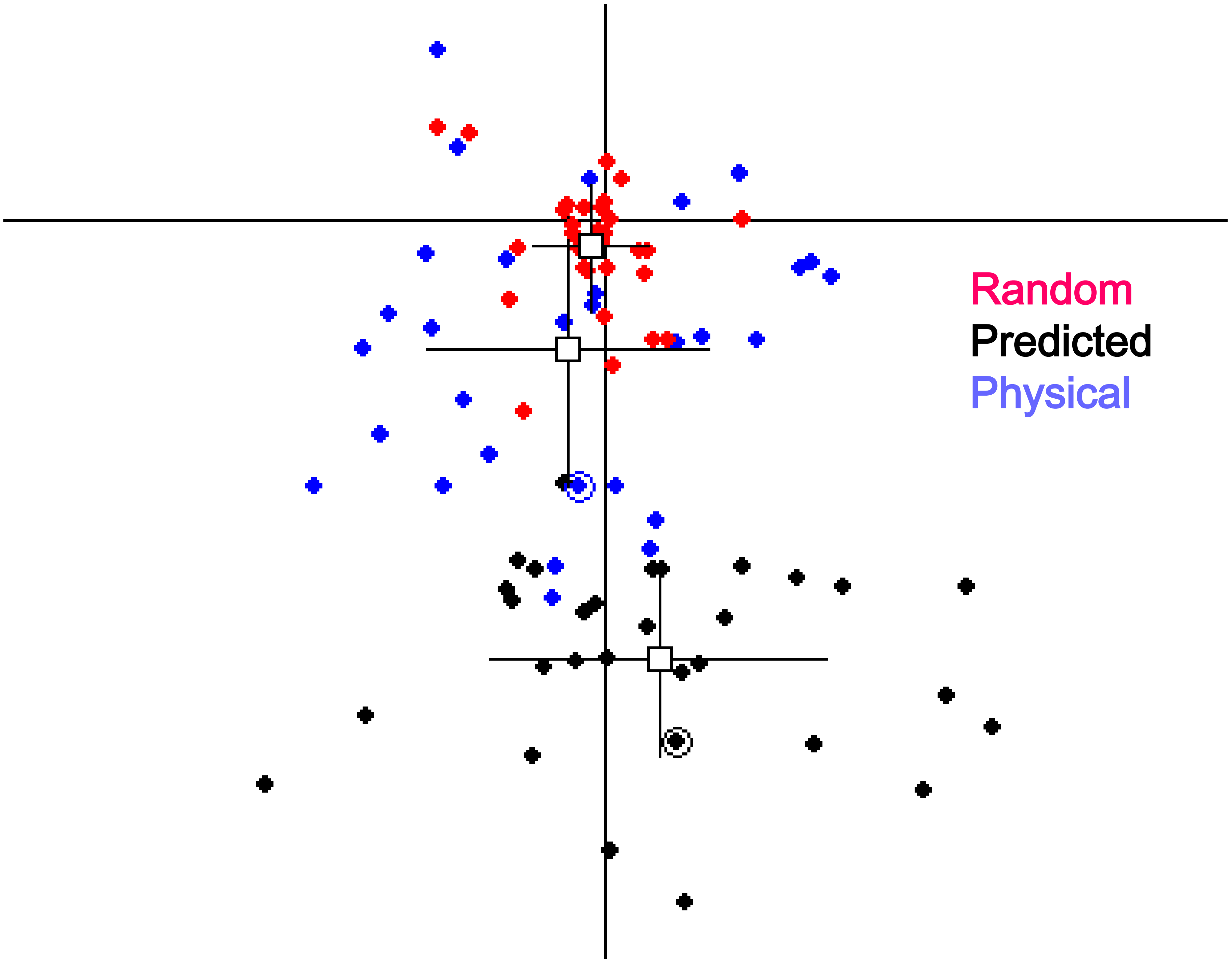


Self-Model synthesis
?
Exploratory Action synthesis

Emergent Self-Model

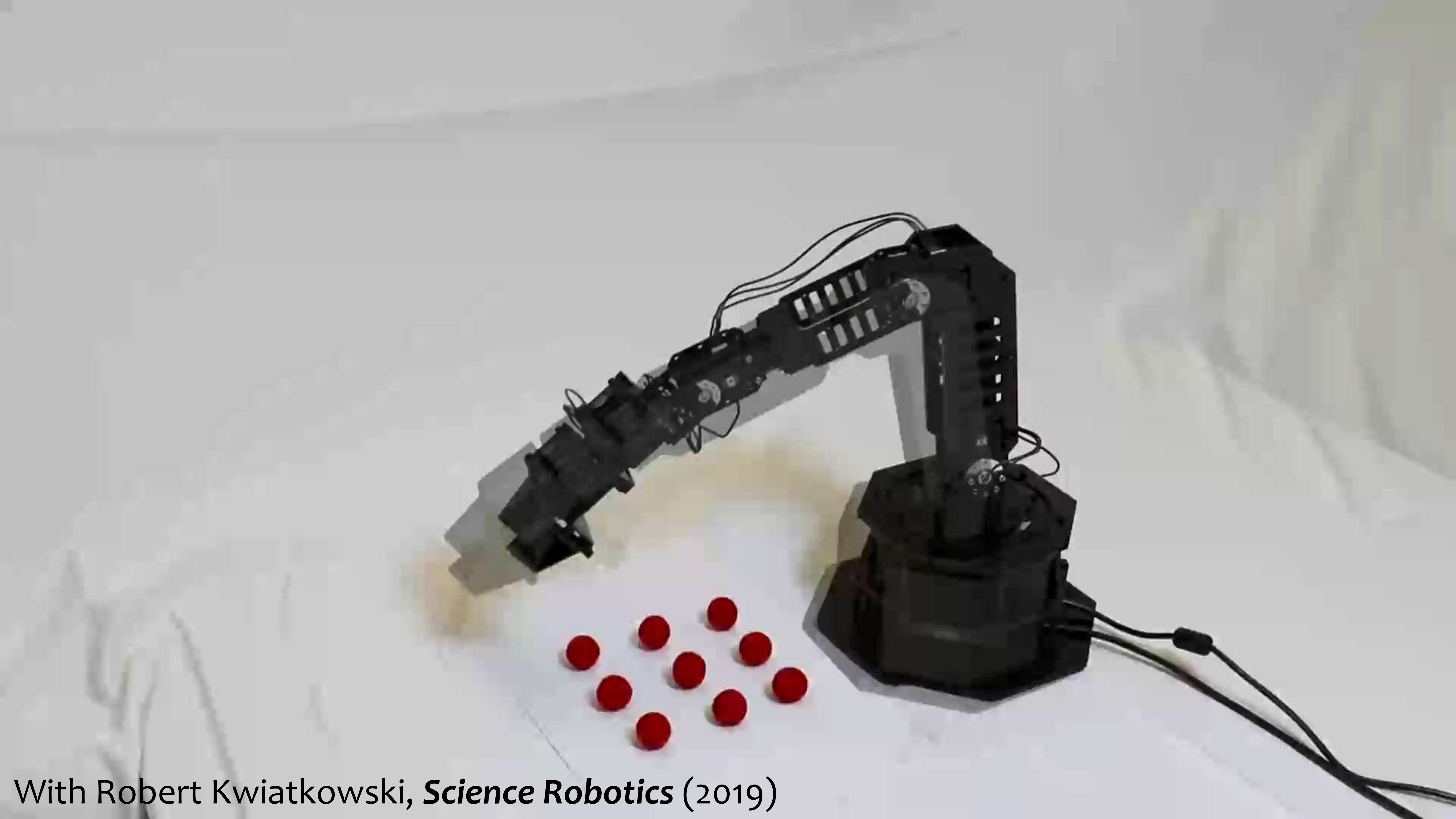
With Josh Bongard and Victor Zykov, ***Science***

With Josh Bongard and Victor Zykov, ***Science***



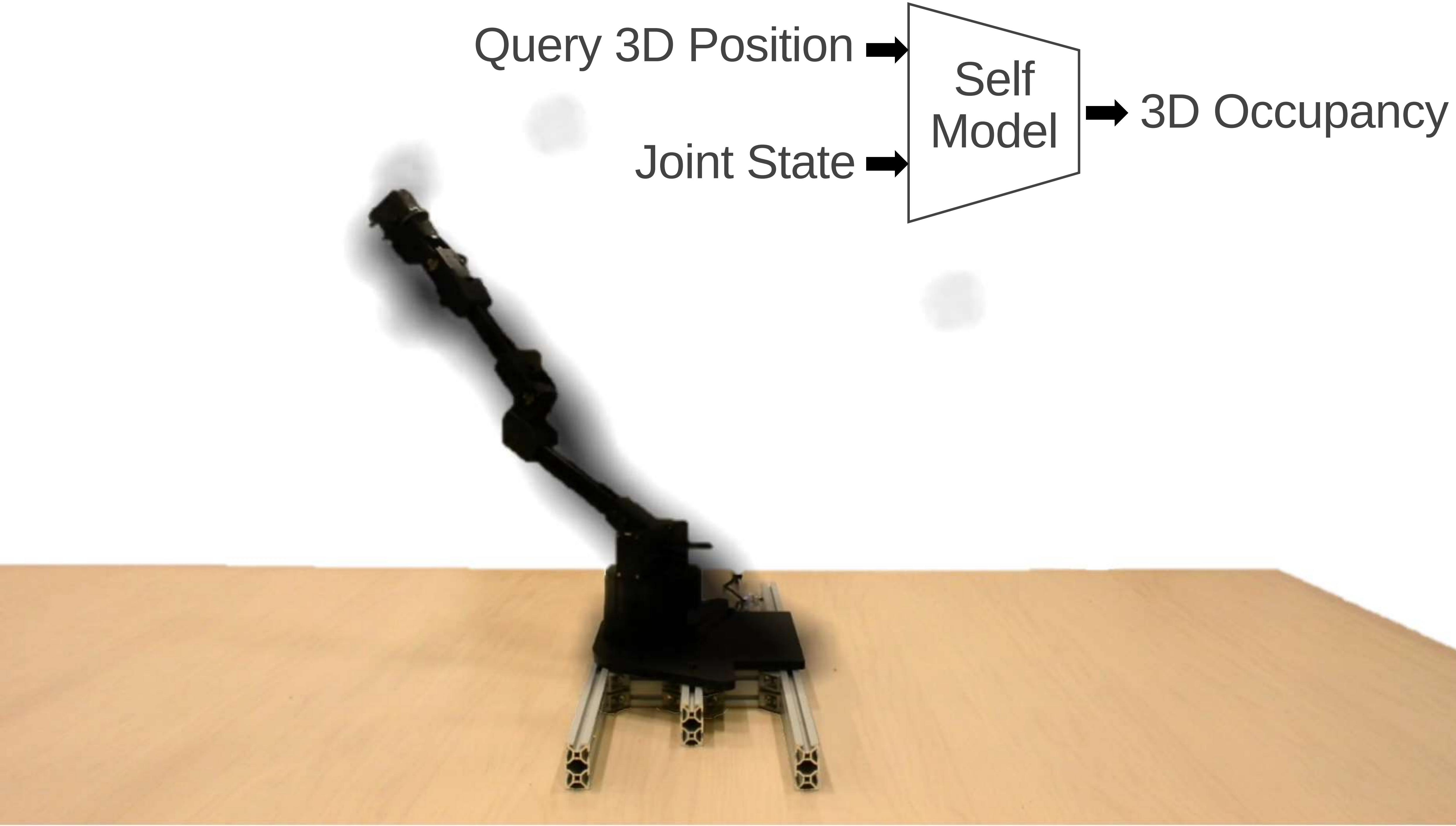
Random
Predicted
Physical

With Robert Kwiatkowski, ***Science Robotics*** (2019)



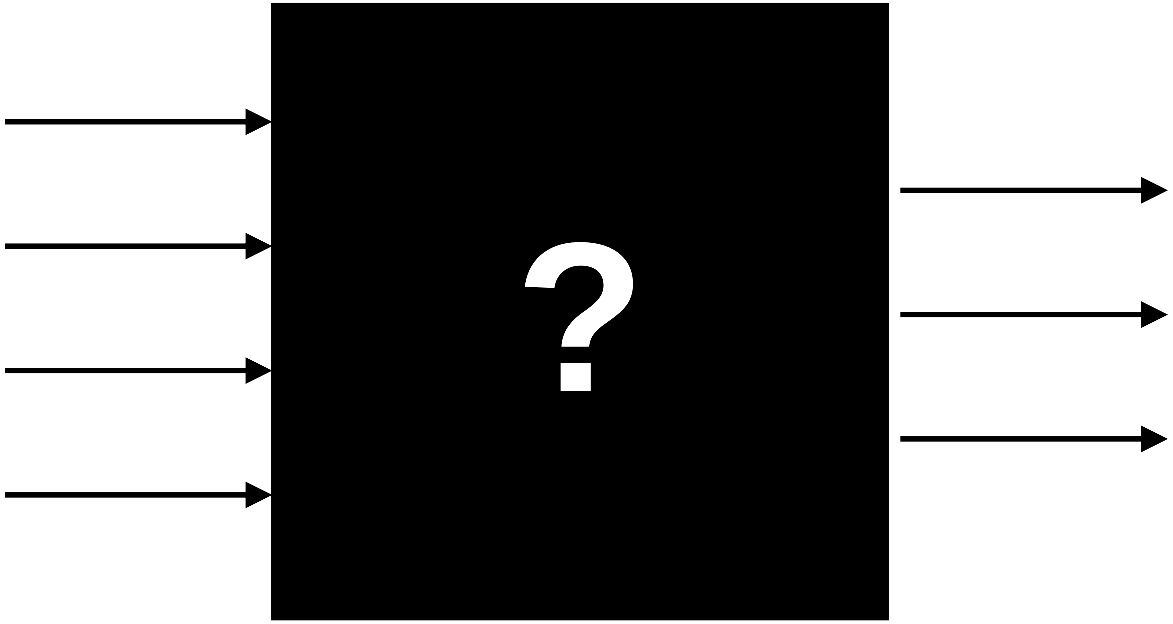
With Robert Kwiatkowski, ***Science Robotics*** (2019)

With Robert Kwiatkowski, ***Science Robotics*** (2019)



Boyuan Chen, Rob Kwiatkowski

System Identification



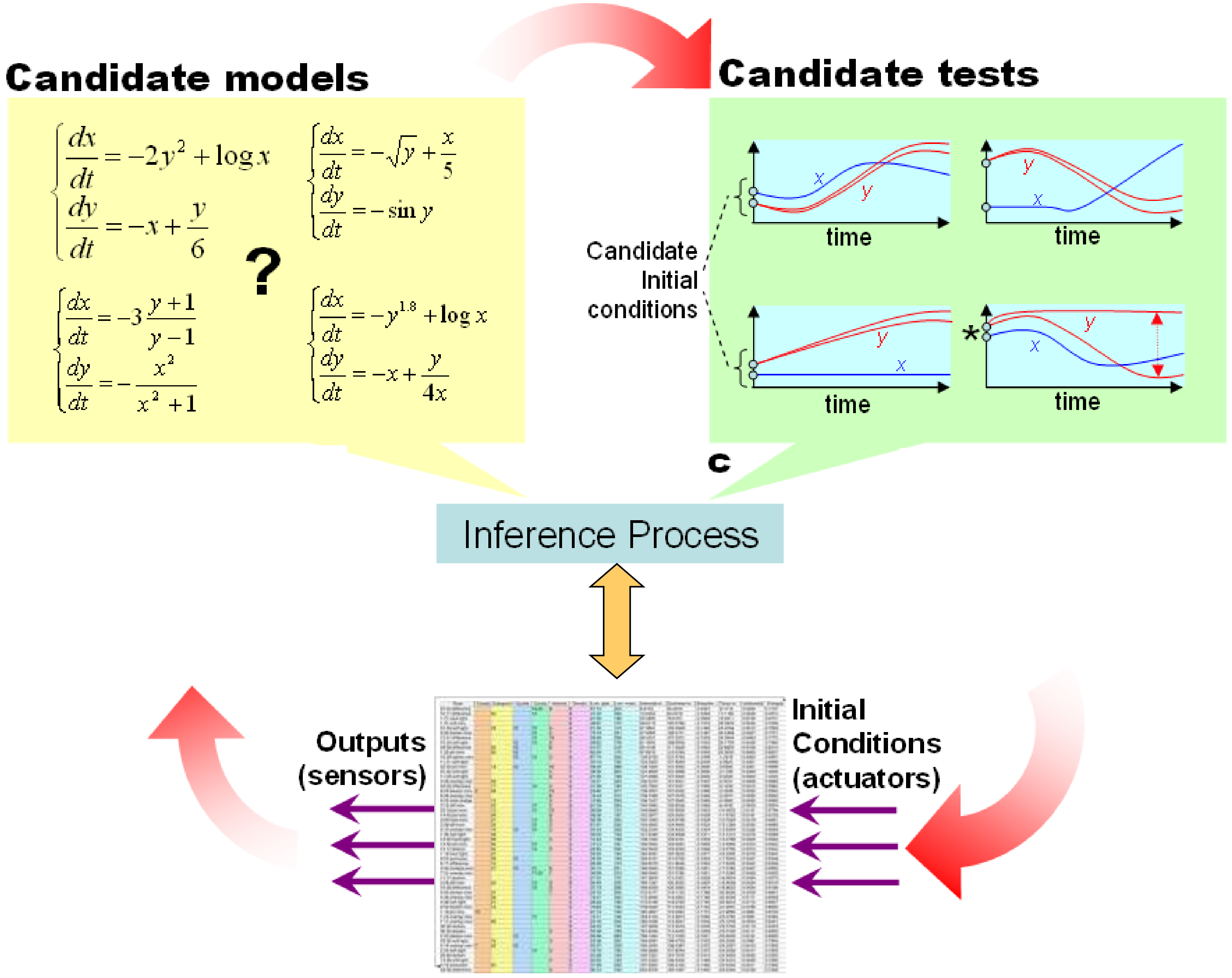
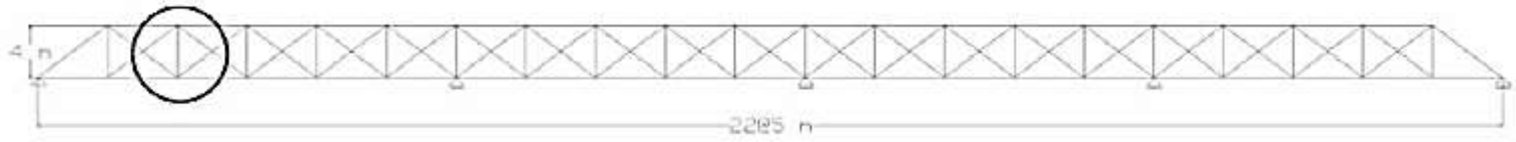
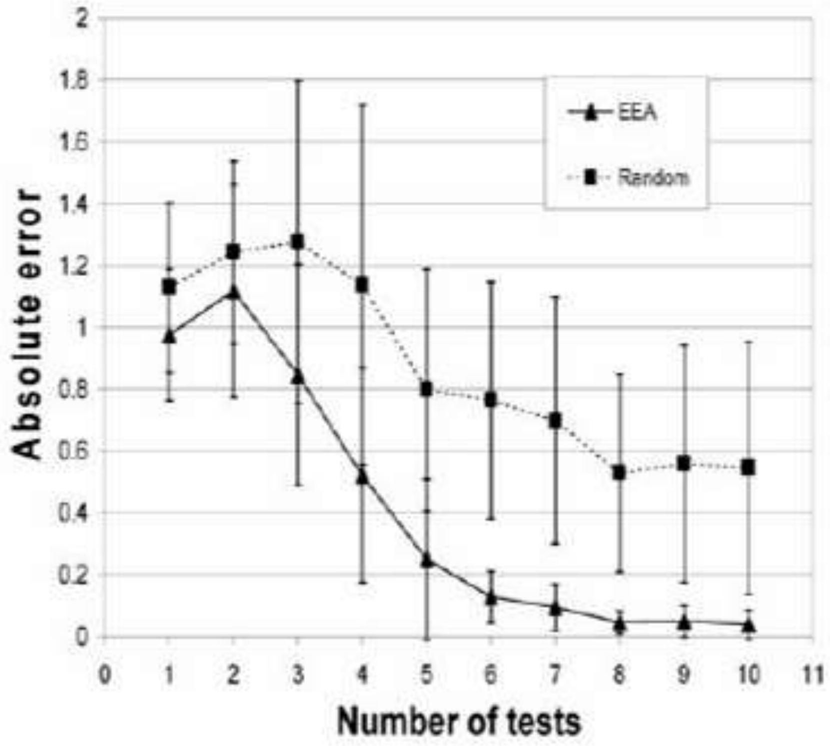

Candidate models
$\frac{dx}{dt} = -2y^2 + \log x$, $\frac{dy}{dt} = -x + \frac{y}{6}$
$\frac{dx}{dt} = -\sqrt{y} + \frac{x}{5}$, $\frac{dy}{dt} = -\sin y$
?
$\frac{dx}{dt} = -3\frac{y+1}{y-1}$, $\frac{dy}{dt} = -\frac{x^2}{x^2+1}$
$\frac{dx}{dt} = -y^{1.8} + \log x$, $\frac{dy}{dt} = -x + \frac{y}{4x}$
Candidate tests
Candidate Initial conditions
x
y
time
*
c
Inference Process
Outputs (sensors)
Initial Conditions (actuators)

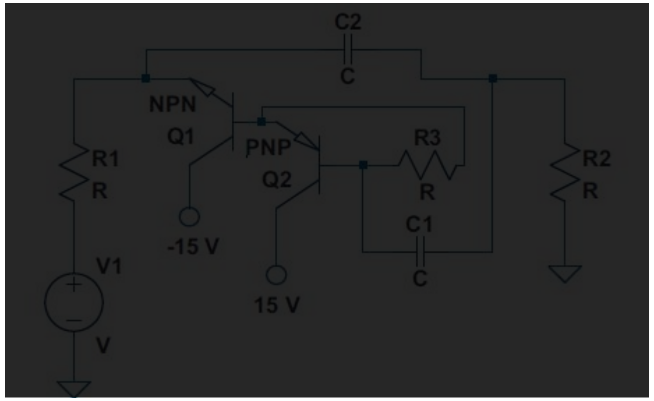
Photo: Floris van Breugel

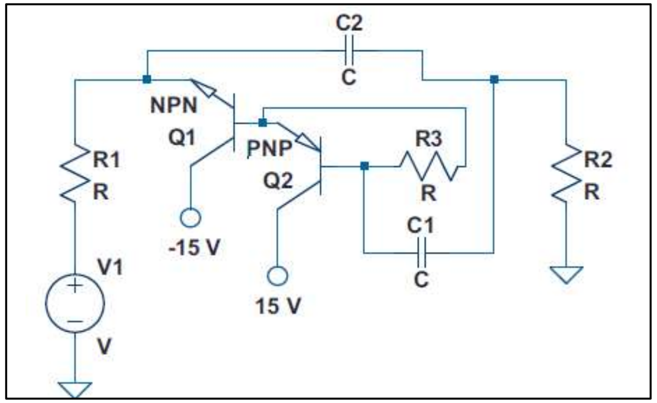
Structural Damage Diagnosis

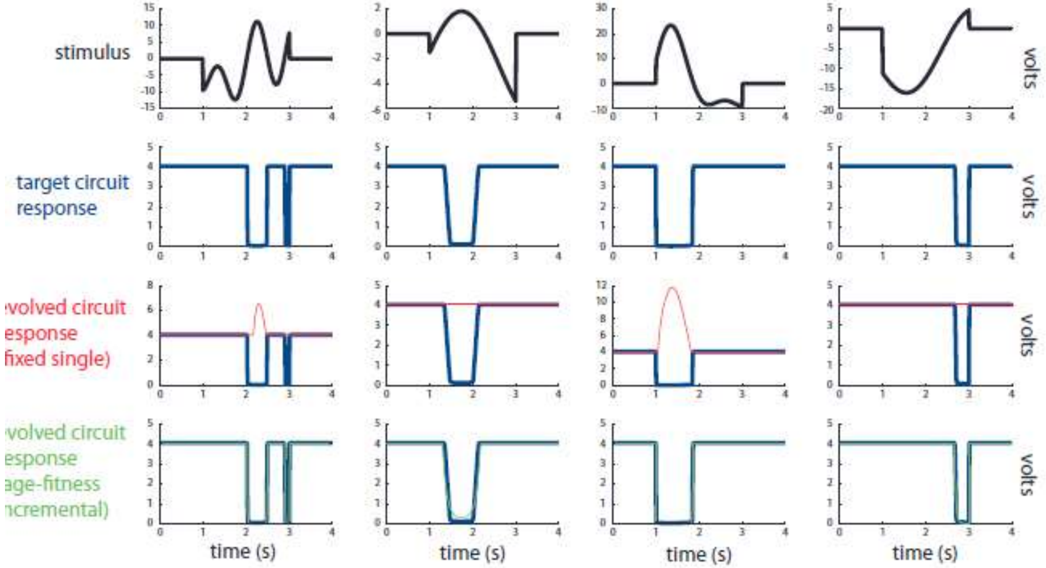




With Wilkins Aquino



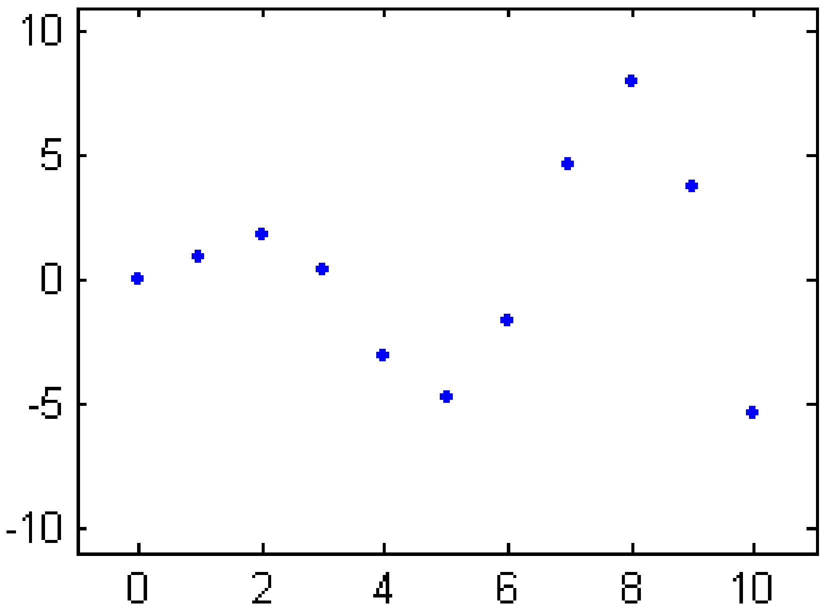


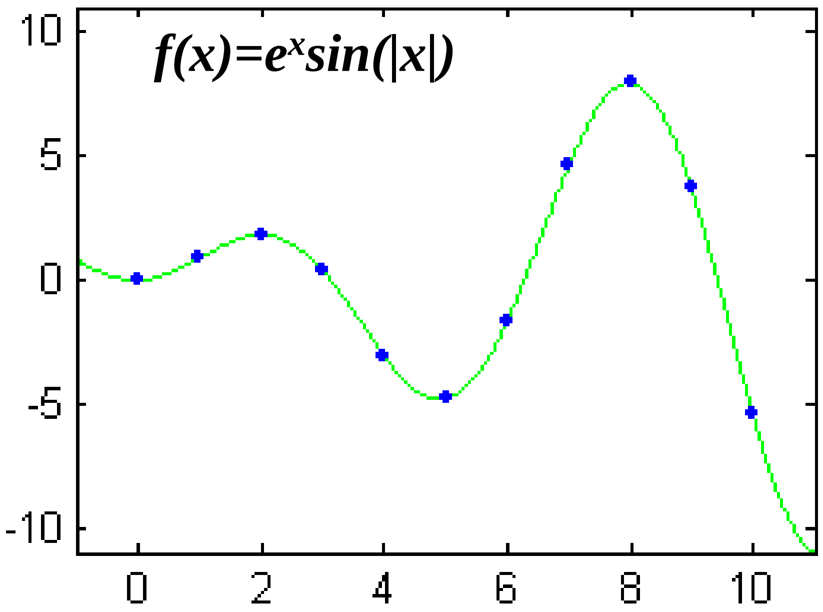


With Ted Cornforth

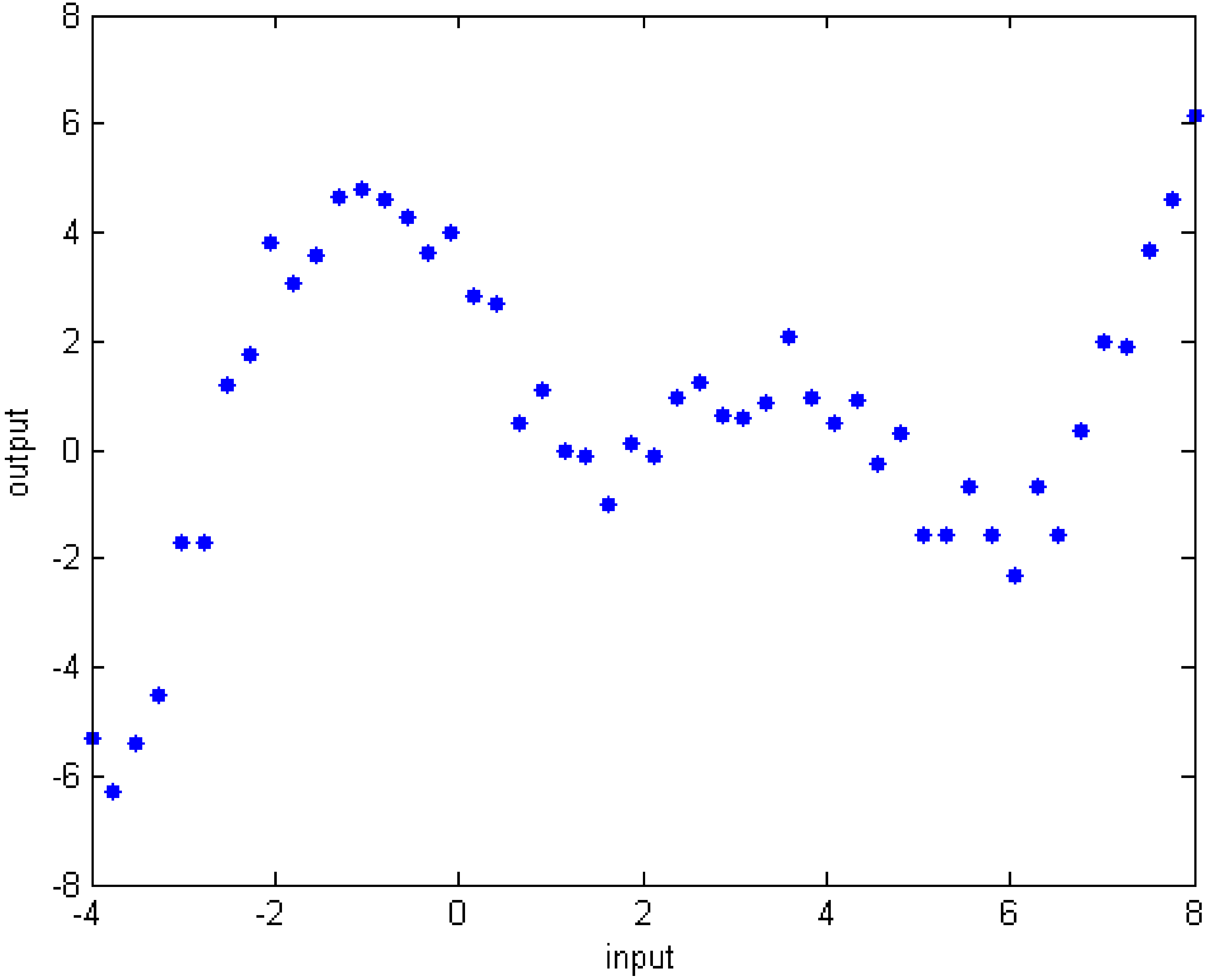
Symbolic Regression

What function describes this data?



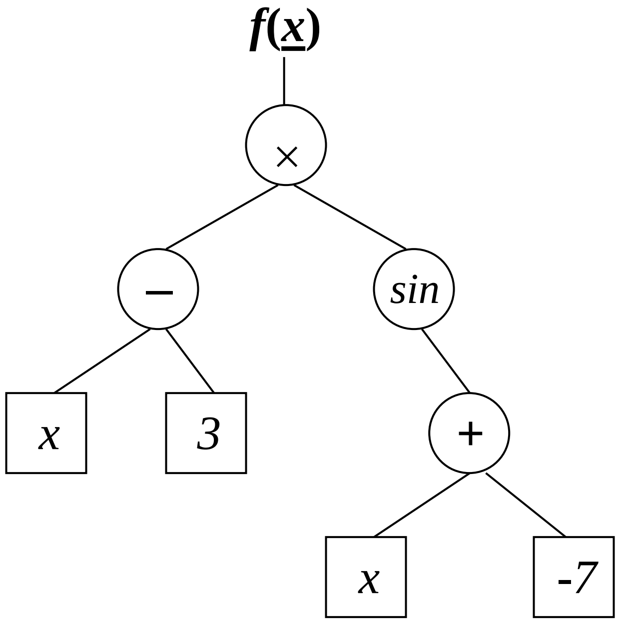


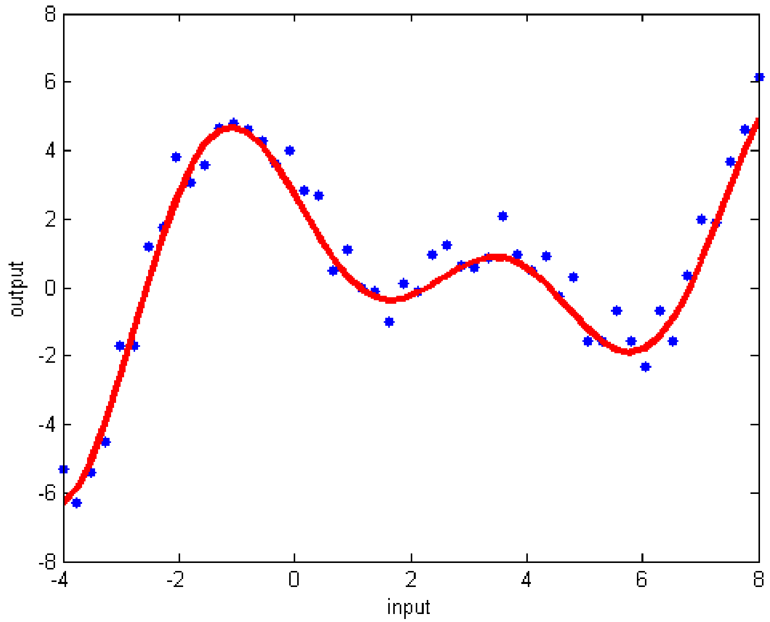
John Koza, 1992


8
6
4
2
0
-2
-4
-6
-8
output
-4
-2
0
2
4
6
8
input

Encoding Equations

Building Blocks: + - * / sin cos exp log … etc





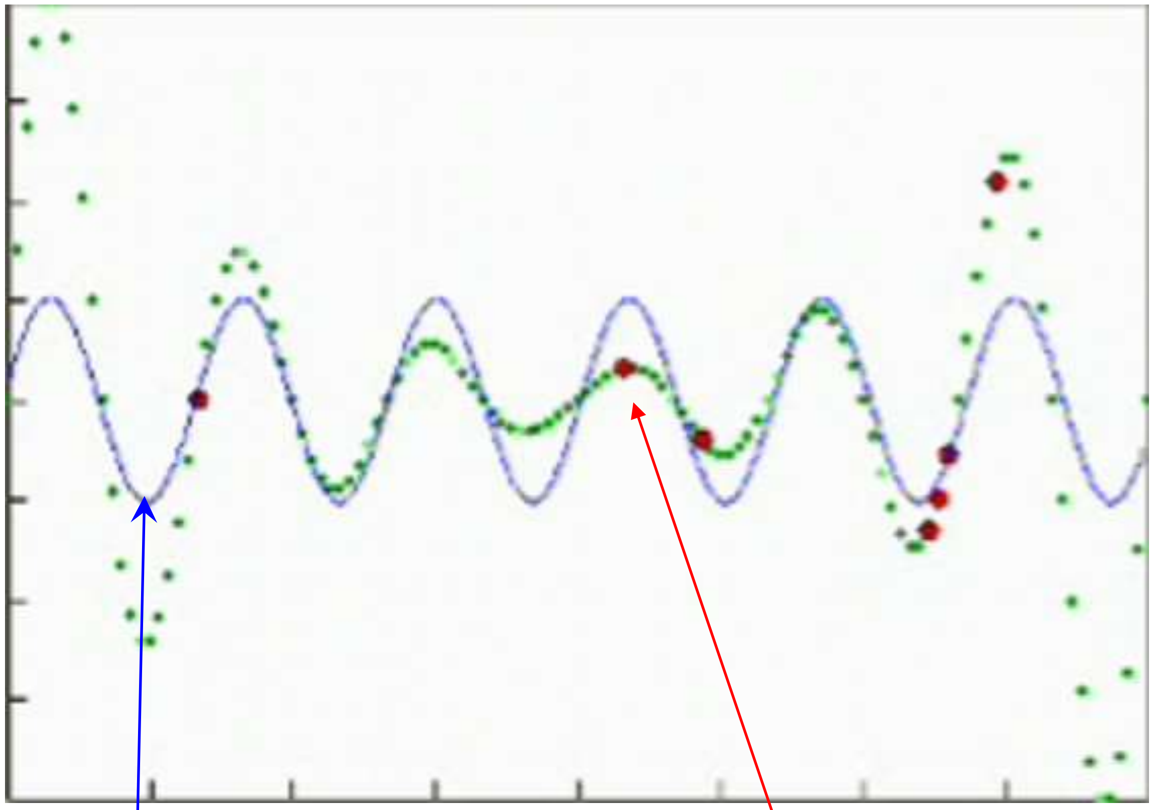
sin(x_2)

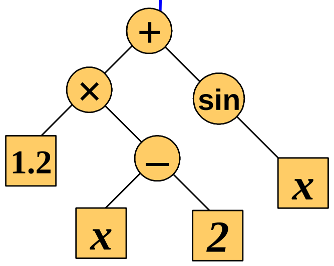
x_1*sin(x_2)

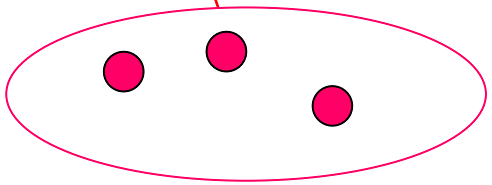
(x_1 – 3)*sin(x_2)

(x_1 – 3)*sin(-7 + x_2)

John Koza, 1992





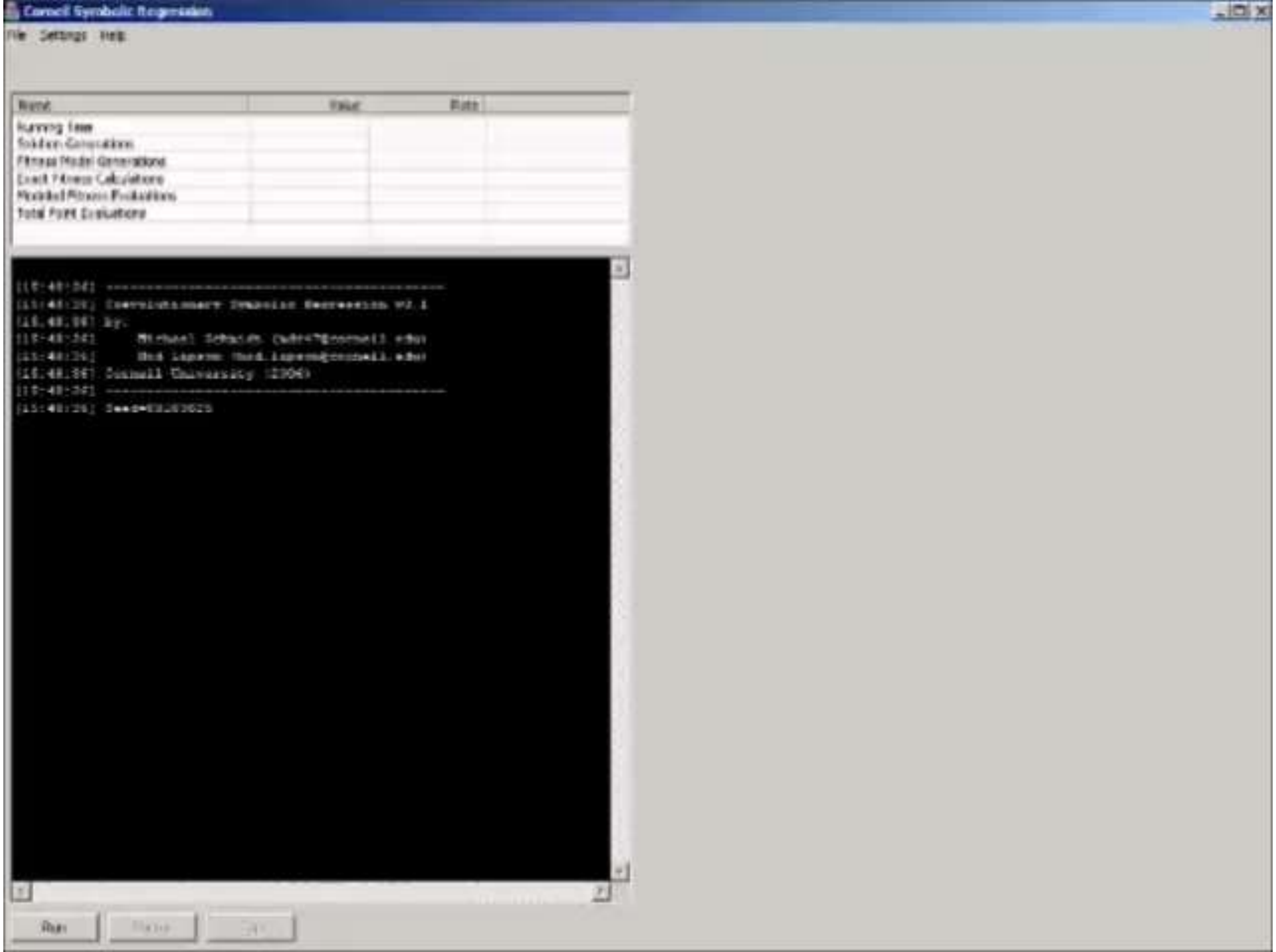


Models: Expression trees
Subject to mutation and selection

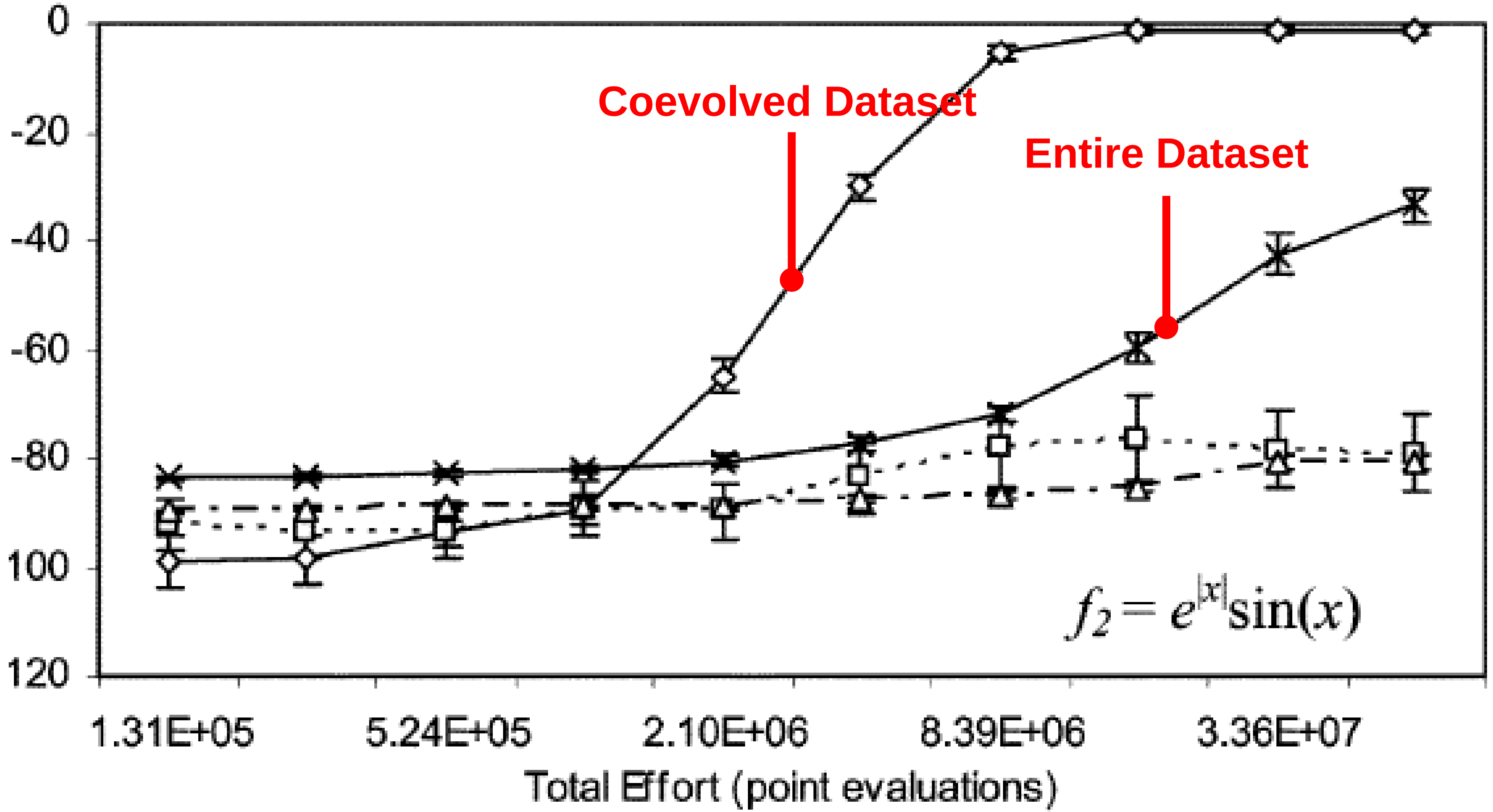
Experiments: Data-points
Subject to mutation and selection

{const,+,-,*,/,sin,cos,exp,log,abs}

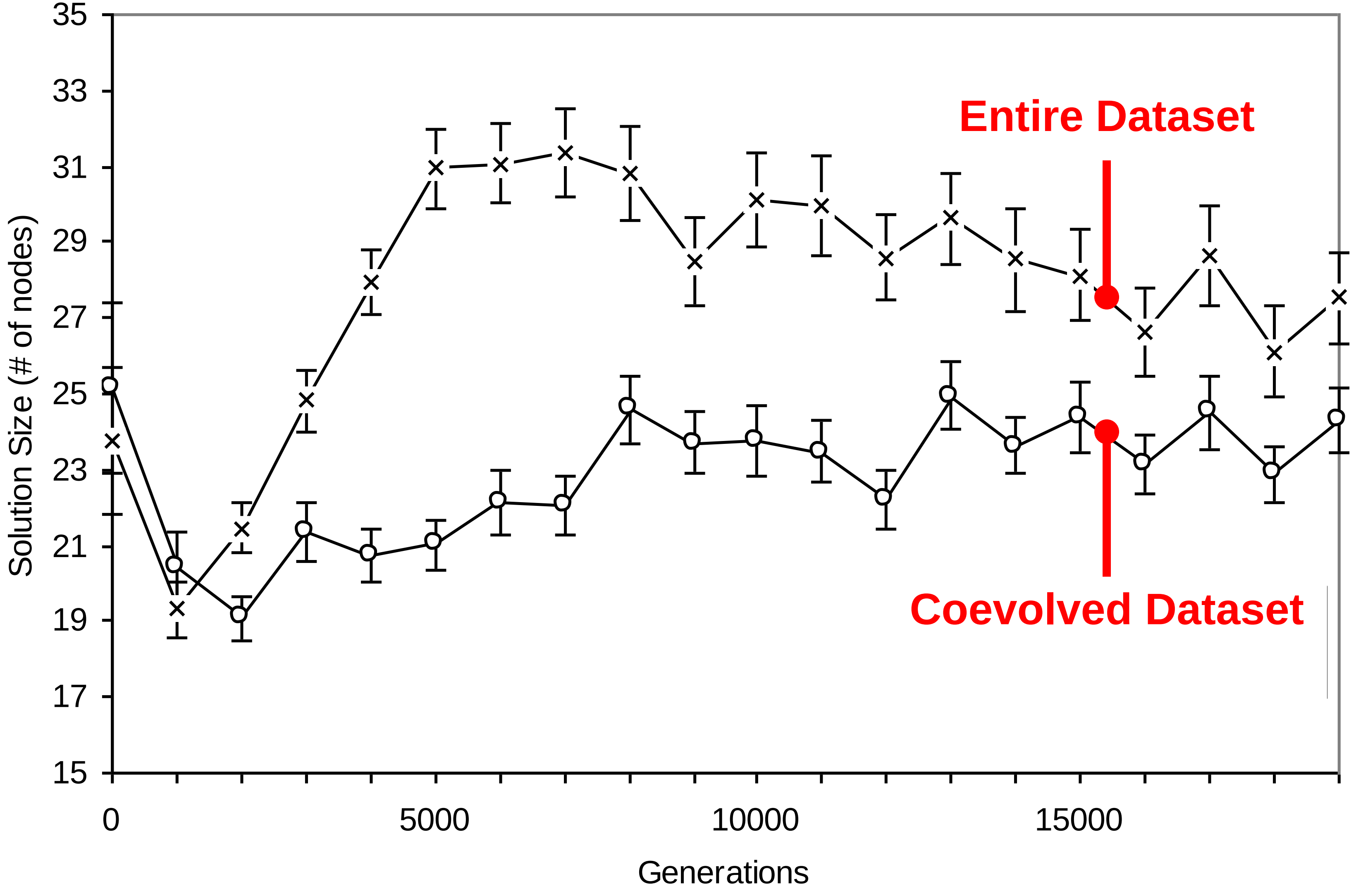
Michael D. Schmidt, Hod Lipson (2006)


Cornell Symbolic Regression
File
Settings
Help
Name
Value
Rate
Running Time
Solution Generations
Fitness Model Generations
Exact Fitness Calculations
Modeled Fitness Evaluations
Total Point Evaluations
Run

Solution Accuracy



Solution Complexity



1	2	3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30
31	32	33	34	35	36	37	38	39	40
41	42	43	44	45	46	47	48	49	50
51	52	53	54	55	56	57	58	59	60
61	62	63	64	65	66	67	68	69	70
71	72	73	74	75	76	77	78	79	80
81	82	83	84	85	86	87	88	89	90
91	92	93	94	95	96	97	98	99	100

Semi-empirical mass formula

Modeling the binding energy of an atomic nucleus

Inferred Formula:

$$E_B = 14.83 - 13.43A + 12.39A^{0.64} + \frac{0.39Z^2}{A^{0.26}} + \frac{17.29(N-Z)^2}{A} \longrightarrow R^2 = 0.99944$$

Weizsäcker's Formula:

$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + \delta(A,Z) \longrightarrow R^2 = 0.999915$$

$$\delta(A,Z) = \begin{cases} +\delta_0 & Z, N \text{ even} \\ 0 & A \text{ odd} \\ -\delta_0 & Z, N \text{ odd} \end{cases} \qquad \delta_0 = \frac{a_P}{A^{1/2}}$$

Systems of Differential Equations

- Regress on derivative

State Variables				*Derivatives*		
time	**x_1**	**x_2**	**…**	**dx_1/dt**	**x_2/dt**	**…**
0	3.4	-1.7	…	-2.0	8.0	…
0.1	3.2	-0.9	…	-1.0	8.0	…
0.2	3.1	-0.1	…	-4.0	1.3	…
0.3	2.7	1.2	…	-5.7	1.9	…
…	…	…	…	…	…	…

Inferring Biological Networks

With Michael Schmidt, John Wikswo Jerry Jenkins

$$\frac{dS_1}{dt} = \underbrace{2.5}_{J_0} - \underbrace{100\left(\frac{S_1 * A_3}{1+13.6769 * A_3^4}\right)}_{-v_1}$$

$$\frac{dS_2}{dt} = \underbrace{200\left(\frac{S_1 * A_3}{1+13.6769 * A_3^4}\right)}_{2*v_1} - \underbrace{6 * S_2 * N_1}_{-v_2} - \underbrace{12 * S_2 * N_1}_{-v_6}$$

$$\frac{dS_3}{dt} = \underbrace{6 * S_2 * N_1}_{v_2} + \underbrace{16 * S_3 * A_2}_{v_3}$$

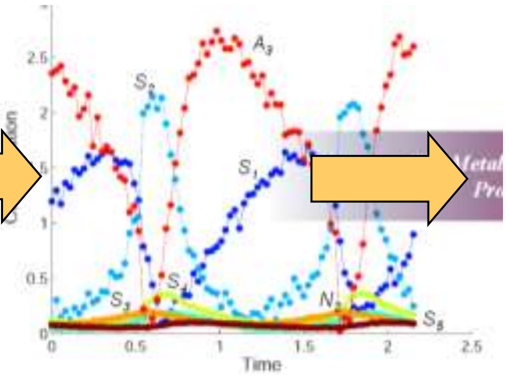
$$\frac{dS_4}{dt} = \underbrace{16 * A_2 * S_3}_{v_3} - \underbrace{100 * N_2 * S_4}_{-v_4}$$

$$\frac{dN_2}{dt} = \underbrace{6 * S_2 * N_1}_{v_2} - \underbrace{100 * N_2 * S_4}_{-v_4}$$

$$\frac{dA_3}{dt} = \underbrace{-200\left(\frac{S_1 * A_3}{1+13.6769 A_3^4}\right)}_{-2*v_1} + \underbrace{32 * A_2 * S_3}_{2v_3} - \underbrace{1.28 * A_3}_{-v_5}$$

$$\frac{dS_5}{dt} = \underbrace{-1.3 * S_5}_{\varphi J}$$

Original Equations



$$\frac{dS_1}{dt} = \underbrace{2.42114}_{J_0} - \underbrace{99.2721\left(\frac{S_1 * A_3}{1+13.5956 * A_3^4}\right)}_{-v_1}$$

$$\frac{dS_2}{dt} = \underbrace{199.935\left(\frac{S_1 * A_3}{1+13.6734 * A_3^4}\right)}_{2*v_1} - \underbrace{5.99475 * S_2 * N_1}_{-v_2} - \underbrace{11.9895 * S_2 * N_1}_{-v_6}$$

$$\frac{dS_3}{dt} = \underbrace{5.99857 * S_2 * N_1}_{v_2} + \underbrace{15.99606 * S_3 * A_2}_{v_3} - \underbrace{0.01286 * S_3}_{extraneous}$$

$$\frac{dS_4}{dt} = \underbrace{15.997 * A_2 * S_3}_{v_3} - \underbrace{100.015 * N_2 * S_4}_{-v_4}$$

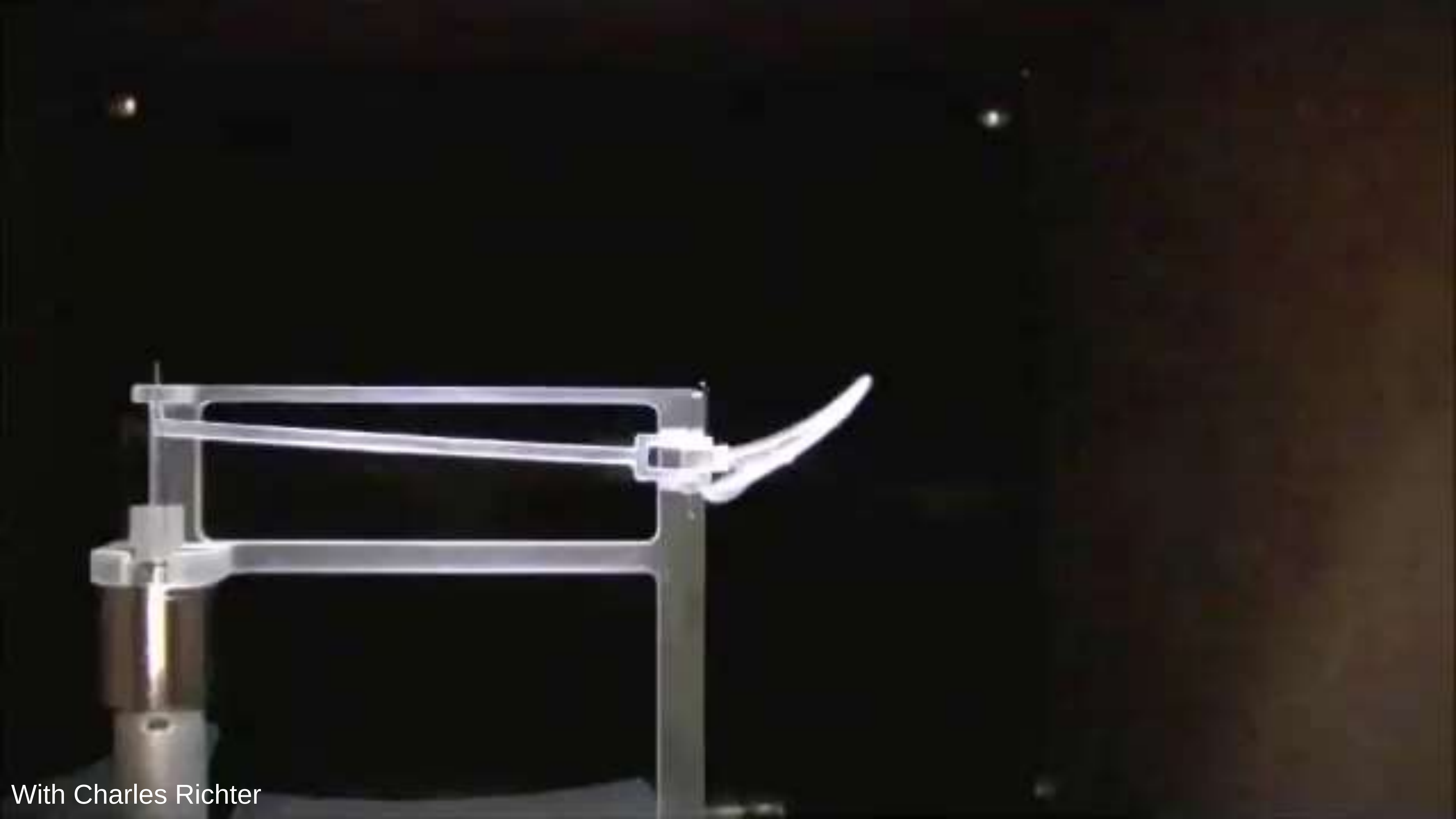
$$\frac{dN_2}{dt} = \underbrace{5.99857 * S_2 * N_1}_{v_2} - \underbrace{99.9963 * N_2 * S_4}_{-v_4}$$

$$\frac{dA_3}{dt} = \underbrace{-197.781\left(\frac{S_1 * A_3}{1+13.2633 A_3^4}\right)}_{-2*v_1} + \underbrace{31.9682 * A_2 * S_3}_{2v_3} - \underbrace{1.29659 * A_3}_{-v_5}$$

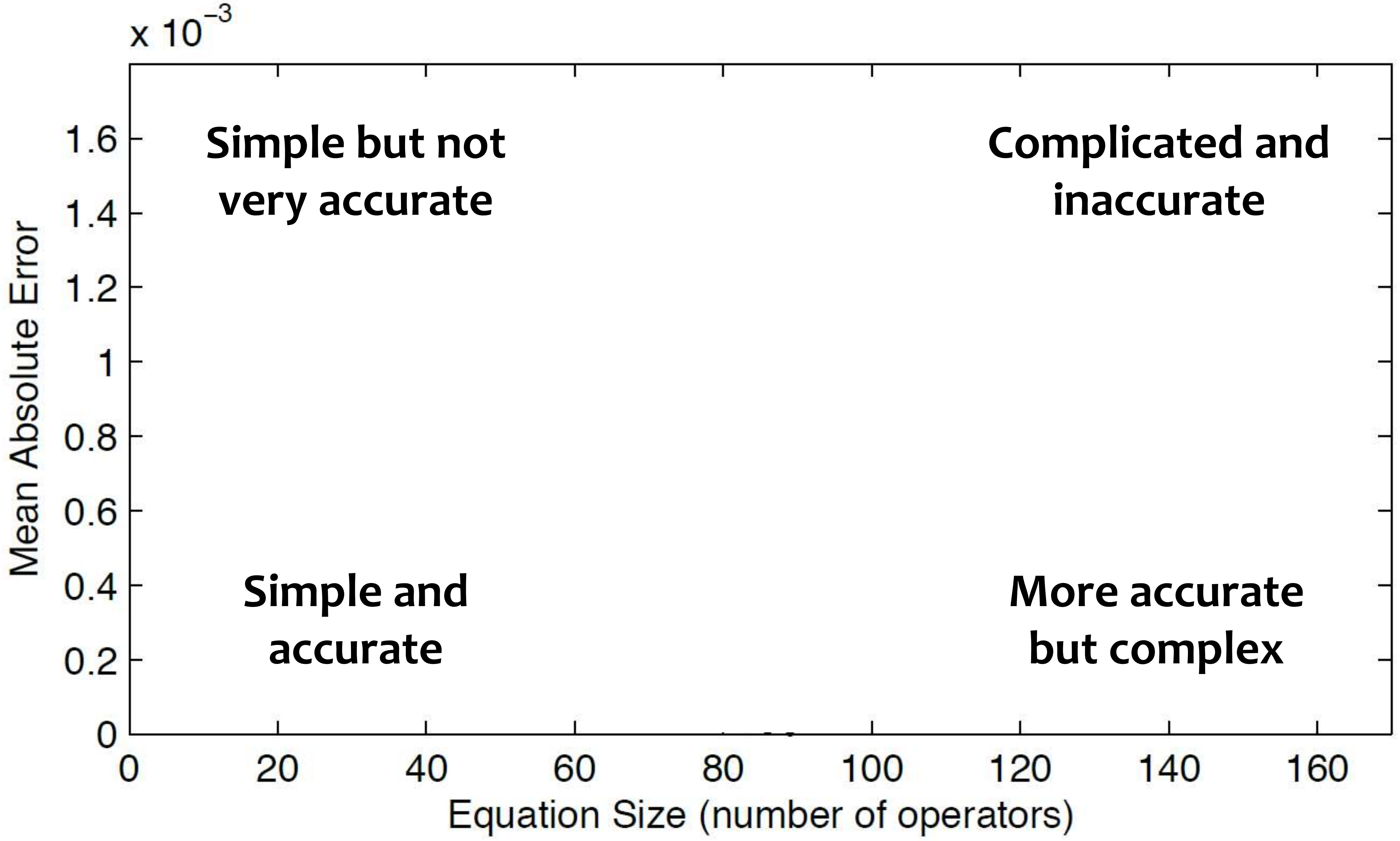
$$\frac{dS_5}{dt} = \underbrace{-1.29626 * S_5}_{\varphi J}$$

Inferred Equations

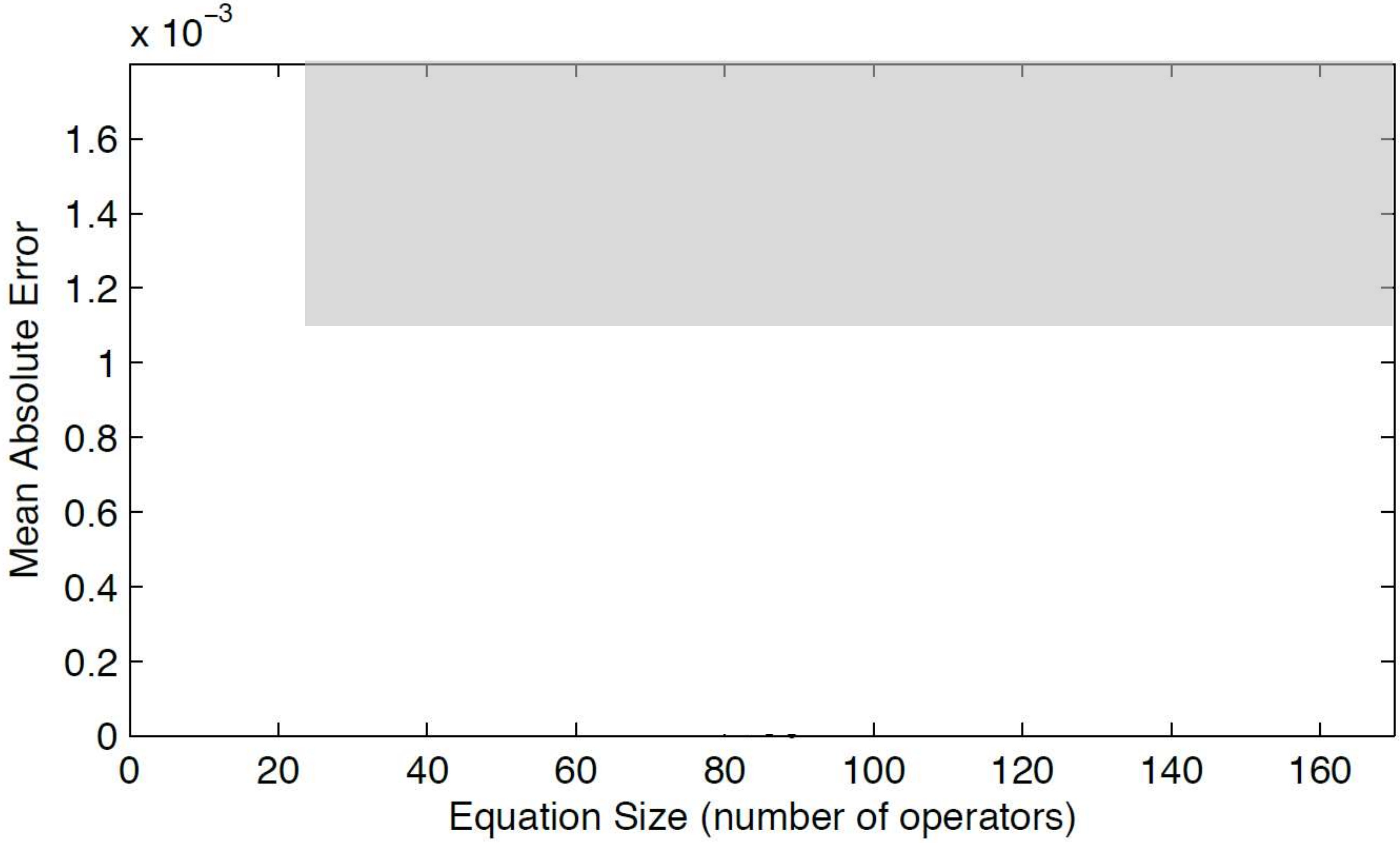
With Charles Richter



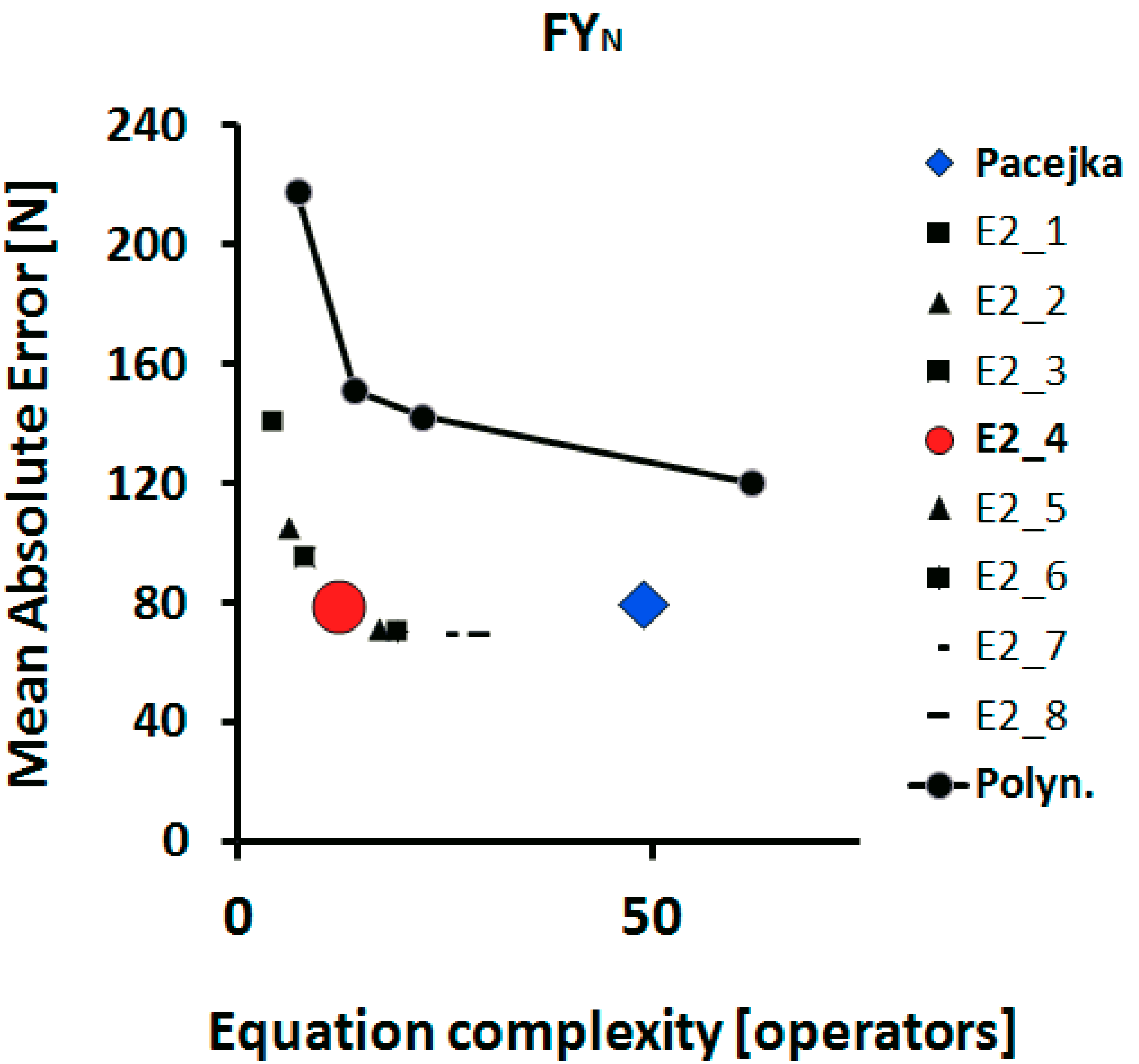
With Charles Richter



With Charles Richter

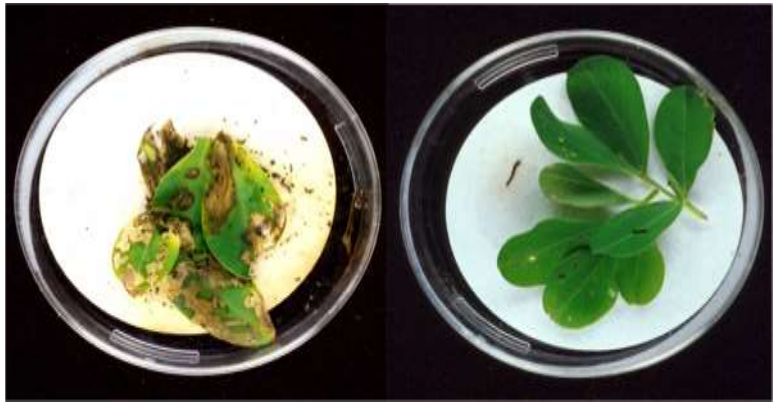


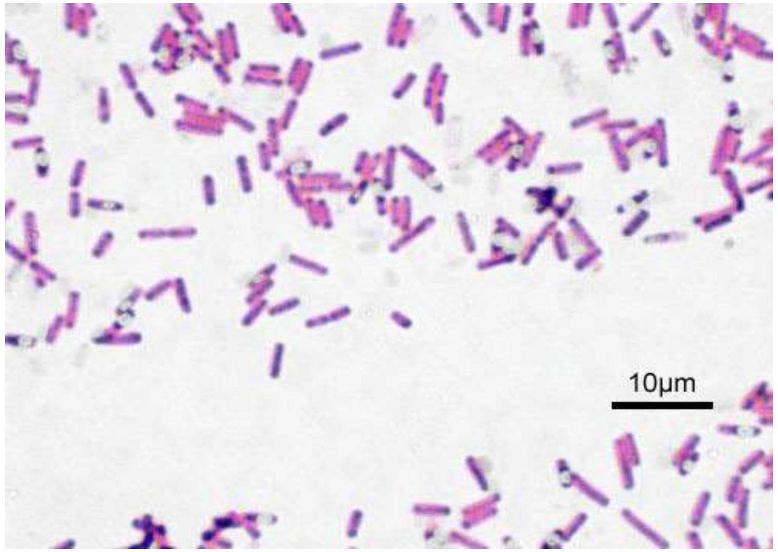
With Charles Richter



Ingmar Zanger, John Amend

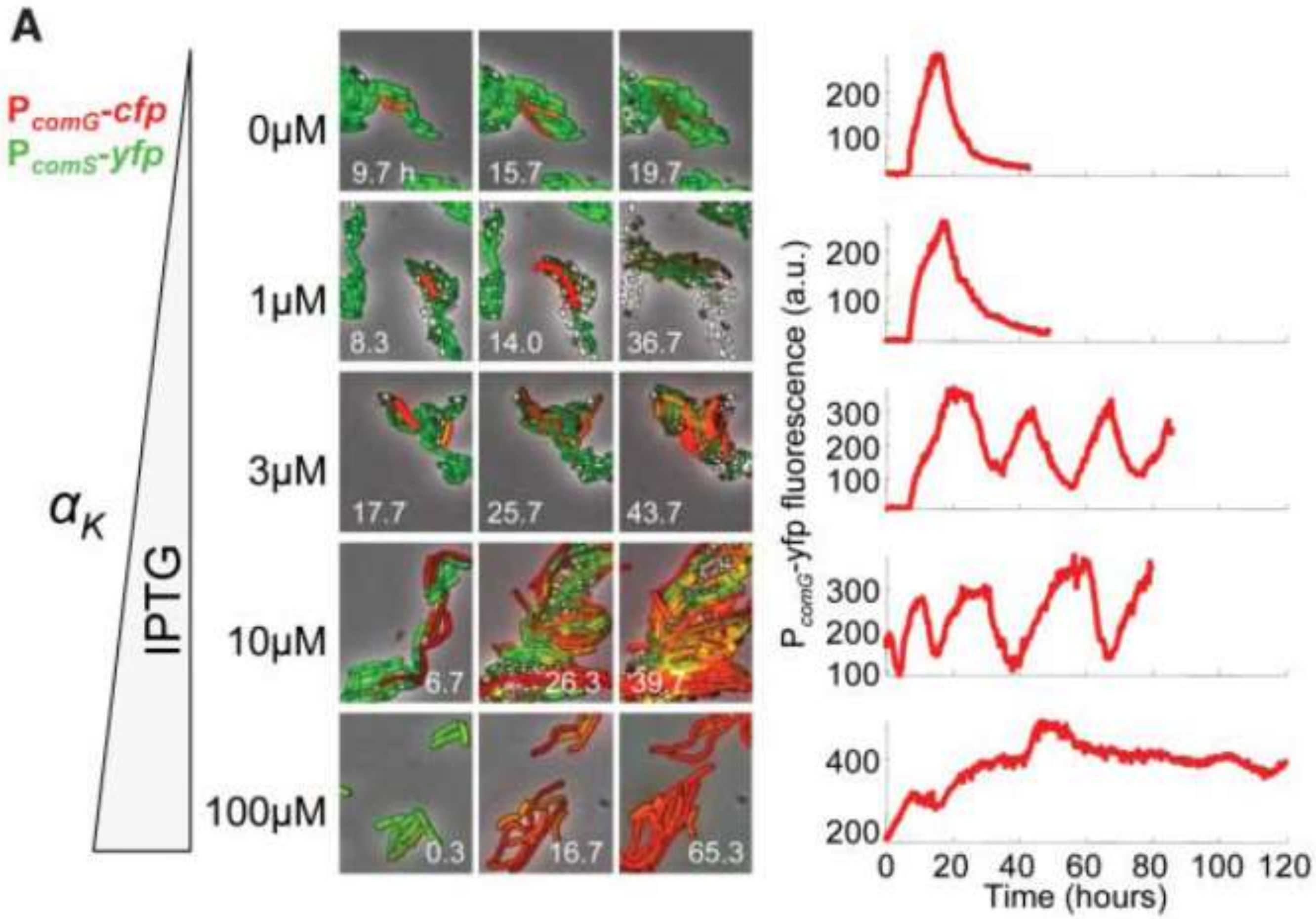
Bacilius Subtilis





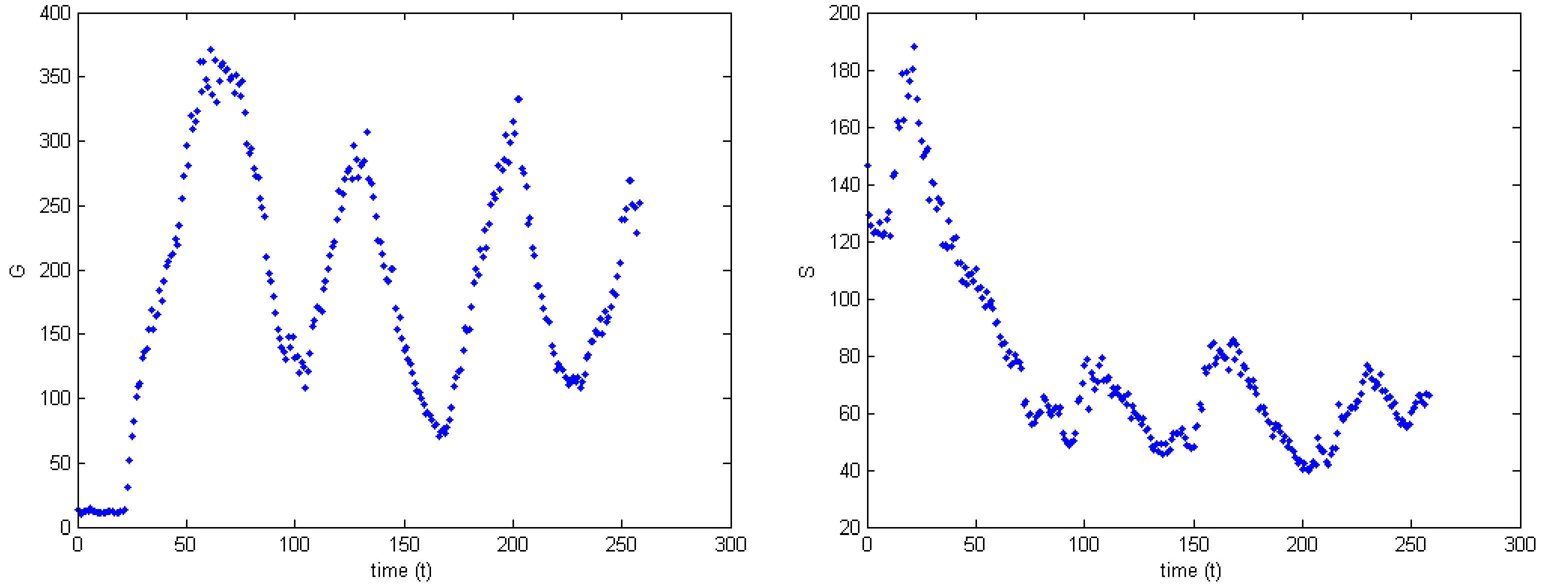
With Michael Schmidt and Gurol Suel

Wet Data, Unknown System

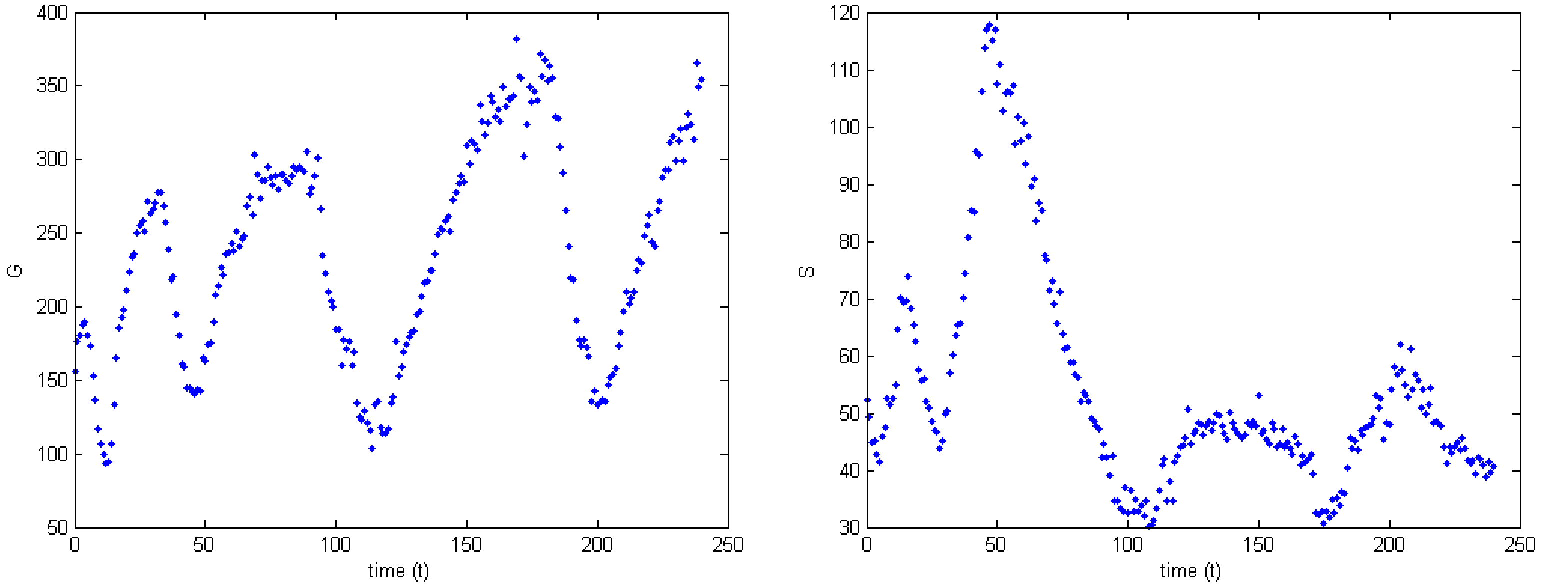


With Michael Schmidt and Gurol Suel

Cell #1



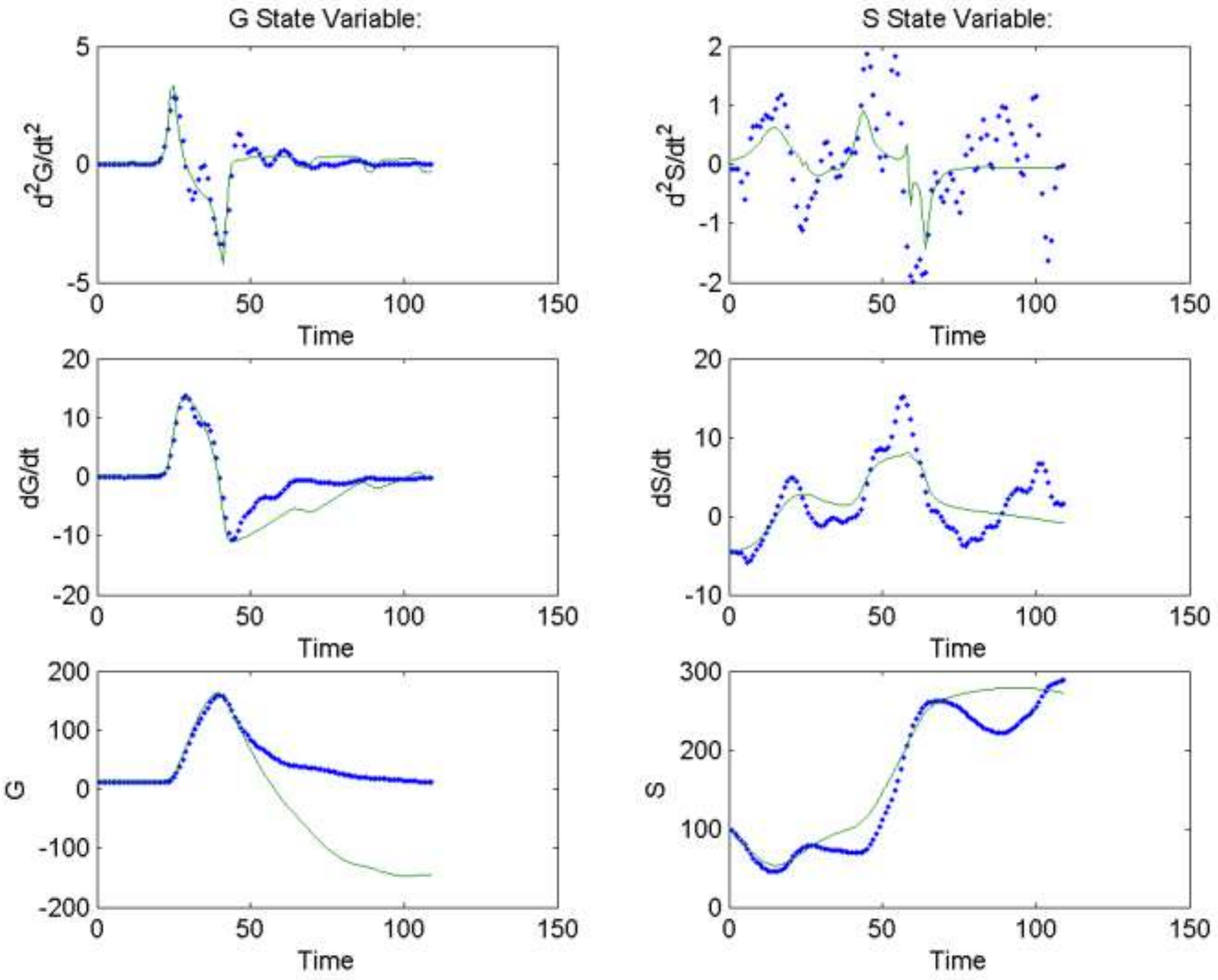
Cell #2



Cell #3-60 …

$$\frac{d^2 G}{dt^2} = 0.329708 - \frac{0.494562\left(G - \frac{dG\,S^2}{(dG-G)^2}\right)}{19.75 + 2\,dG + e^{\frac{dG\,S}{dG-G}}}$$

$$\frac{d^2 S}{dt^2} = -0.0949 + \frac{0.511803}{-36.951 + 4\,dG + G} + \frac{13.1334 - 1.46\,dG}{-1.42633\,(18.96 - dG) + S}$$



Blue Dots = data points, Green Line = regressed fit

Symbolic Regression Inferred *Time-Delay* Model:

$$\frac{dK}{dt} = a_K + \frac{b_K + c_K S}{K}$$

$$\frac{dS}{dt} = a_S + \frac{b_S + c_S K}{S}$$

Biologist's Inferred Model: Gurol Suel, et. al., Science

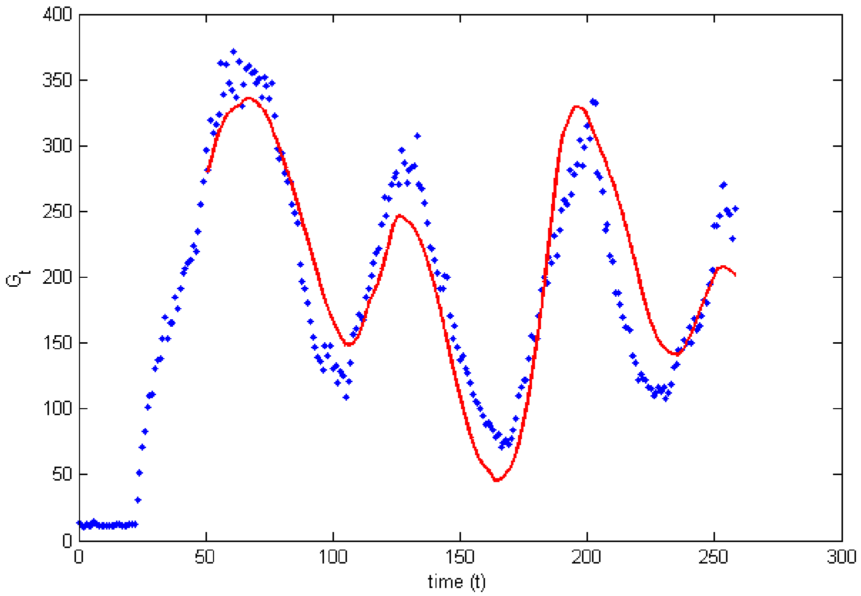
$$\frac{d\boldsymbol{K}}{d\boldsymbol{t}} = \alpha_k + \frac{\beta_K \boldsymbol{K}^n}{\boldsymbol{k}_0^n + \boldsymbol{K}^n} - \frac{\delta_K \boldsymbol{K}}{1 + \boldsymbol{K} / \Gamma_K + \boldsymbol{S} / \Gamma_S} - \lambda_K \boldsymbol{K}$$

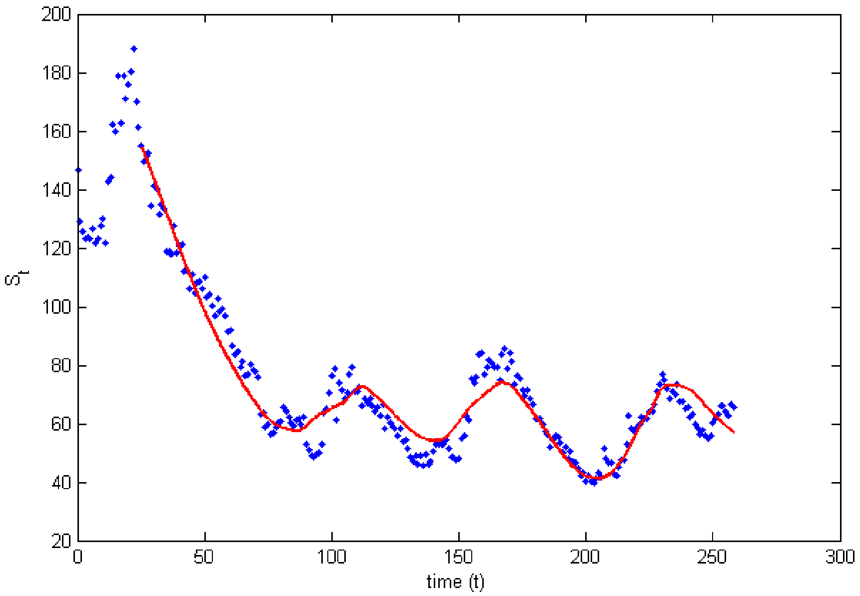
$$\frac{d\boldsymbol{S}}{d\boldsymbol{t}} = \alpha_S + \frac{\beta_S}{1 + \left(\boldsymbol{K} / \boldsymbol{k}_1\right)^p} - \frac{\delta_k \boldsymbol{S}}{1 + \boldsymbol{K} / \Gamma_K + \boldsymbol{S} / \Gamma_S} - \lambda_S \boldsymbol{S}$$

Withheld Test Set #1 Fit

$$\frac{dG_t}{dt} = \frac{1582.0 + 17.3214 \cdot S_{t-51}}{G_{t-18}} - 16.7423$$

$$\frac{dS_t}{dt} = \frac{114.922 + 0.3019 \cdot G_{t-25}}{S_{t-15}} - 3.05$$

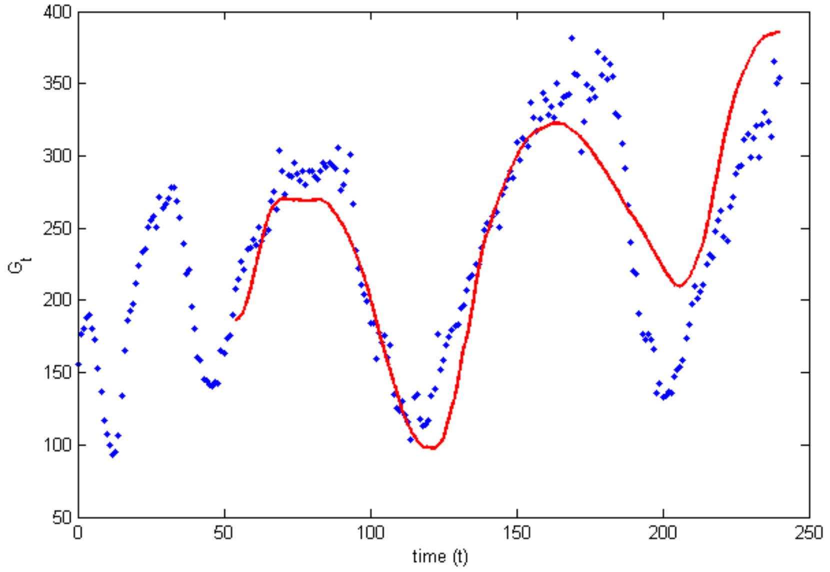


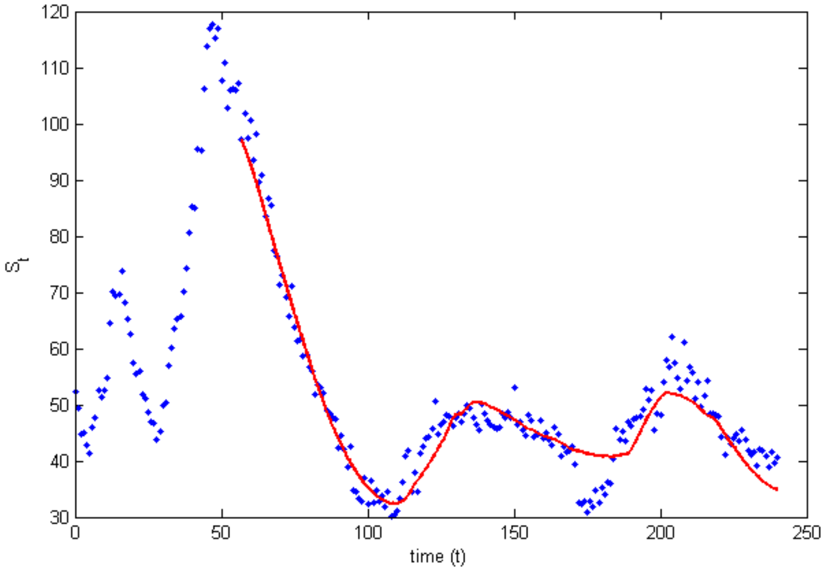


Withheld Test Set #2 Fit

$$\frac{dG_t}{dt} = \frac{3526.92 - 21.312 \cdot S_{t-54}}{G_{t-17}} - 10.1355$$

$$\frac{dS_t}{dt} = \frac{132.271 - 0.0178 \cdot G_{t-57}}{S_{t-18}} - 2.9693$$

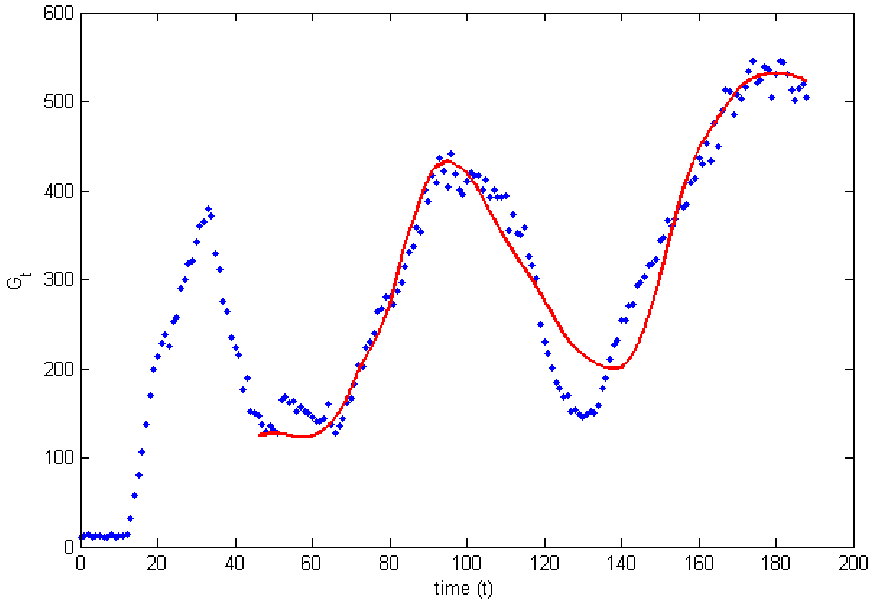


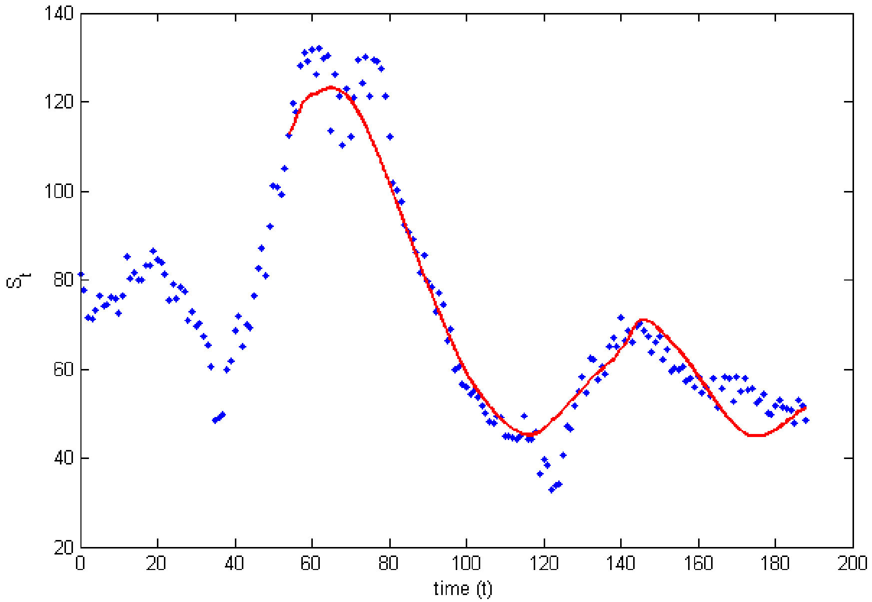


Withheld Test Set #3 Fit

$$\frac{dG_t}{dt} = \frac{5057.1 - 39.7452 \cdot S_{t-46}}{G_{t-21}} - 6.4406$$

$$\frac{dS_t}{dt} = \frac{295.426 - 0.2965 \cdot G_{t-54}}{S_{t-20}} - 3.871$$

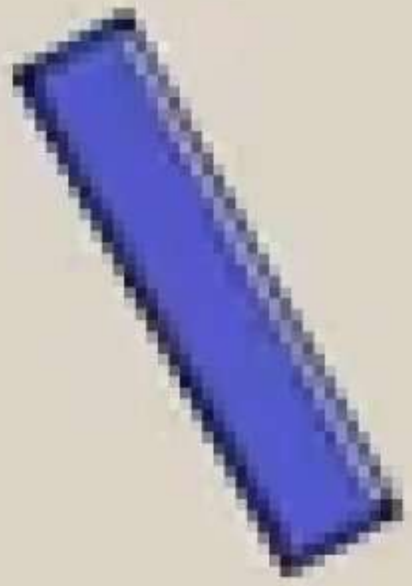





Searching for meaning

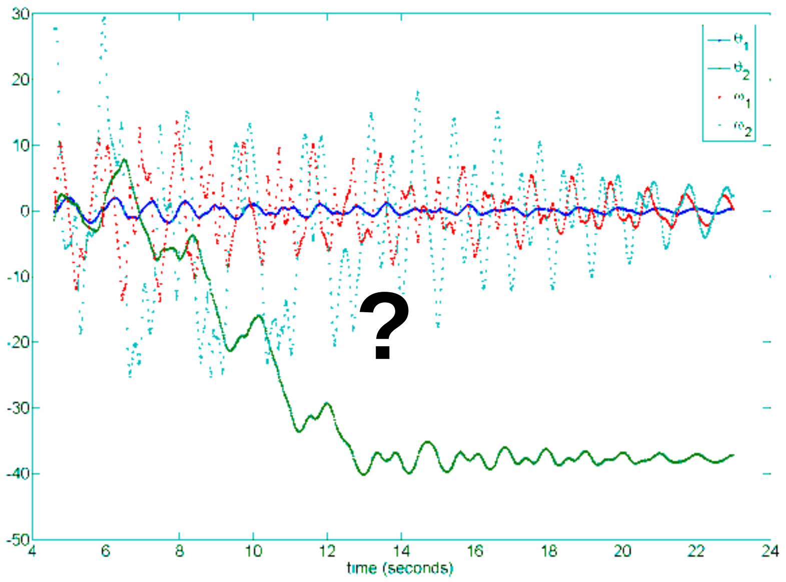
Correlations

θ_t , ω_t



$$f(\theta_t , \omega_t)=const$$

https://gfycat.com/understateddefenselessarrowana-experimento-pendulum-physics-fisica



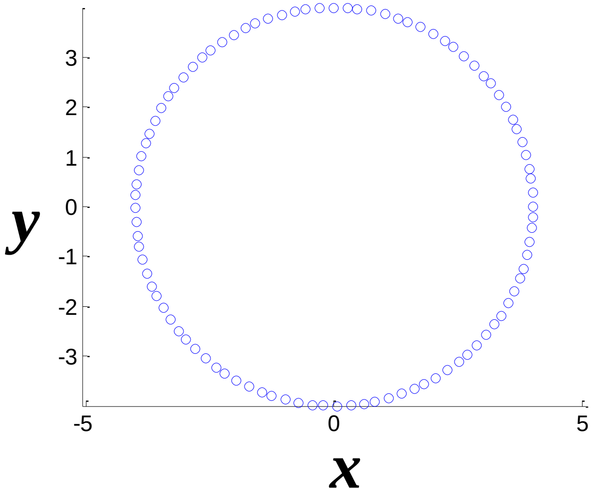
42

42+x–x

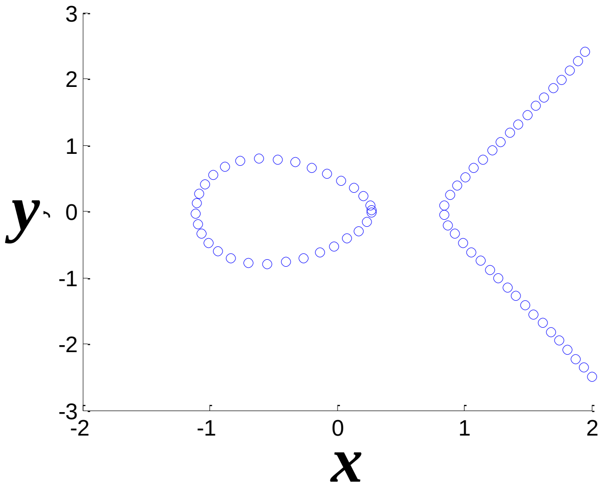
42+x/1000

Homework

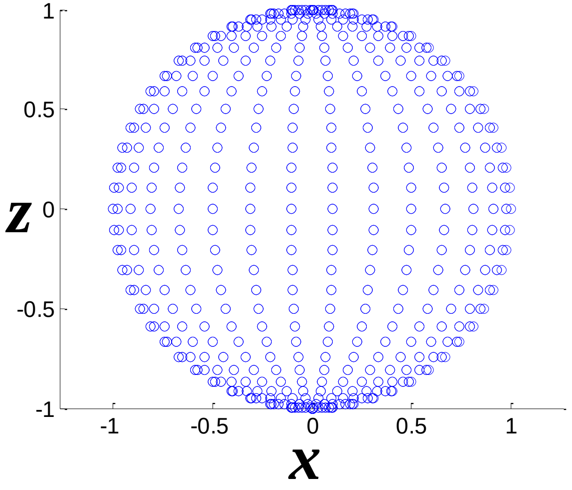
Circle



Elliptic Curve



Sphere



$x^2 + y^2 - 16 = 0$

$x^3 + x - y^2 - 1.5 = 0$

$x^2 + y^2 + z^2 - 1 = 0$

From Data:

x	y	…
0.1	2.3	
0.2	4.5	
0.3	9.7	
0.4	5.1	
0.5	3.3	
0.6	1.0	
…	…	…

Calculate partial derivatives Numerically:

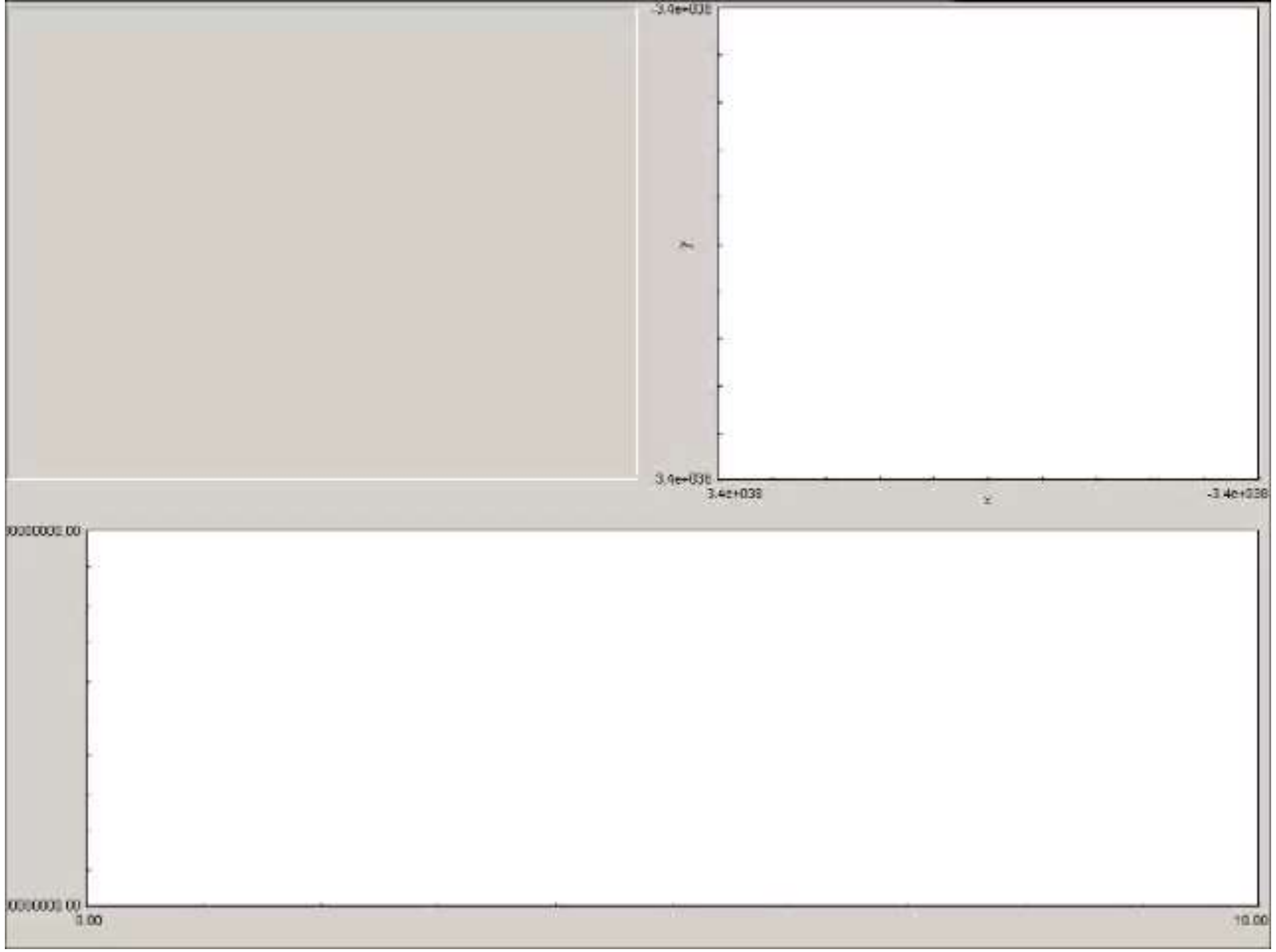
$$\longrightarrow \quad \frac{\delta x}{\delta y}, \quad \frac{\delta y}{\delta x}, \quad \ldots$$

From Equation:

Calculate predicted partial derivatives Symbolically:

$$\frac{\delta f}{\delta x} \Big/ \frac{\delta f}{\delta y} \quad \longrightarrow \quad \frac{\delta x'}{\delta y'}, \quad \frac{\delta y'}{\delta x'}, \quad \ldots$$

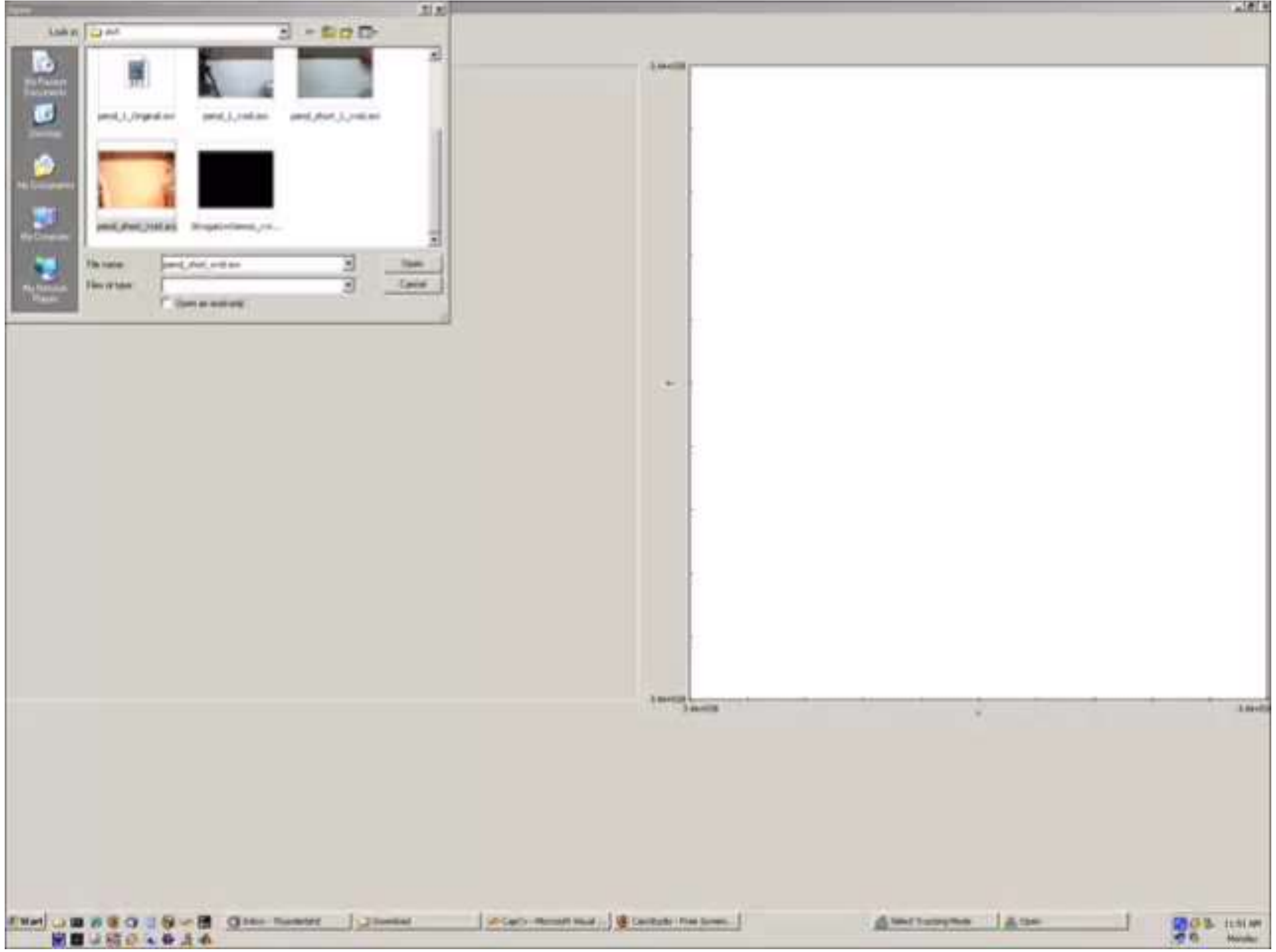
Linear Oscillator



$$H = 114.28 * \left(\frac{dx}{dt} \right)^2 + 692.322 * x^2$$

$$L = 61.591 * \left(\frac{dx}{dt} \right)^2 - 369.495 * x^2$$

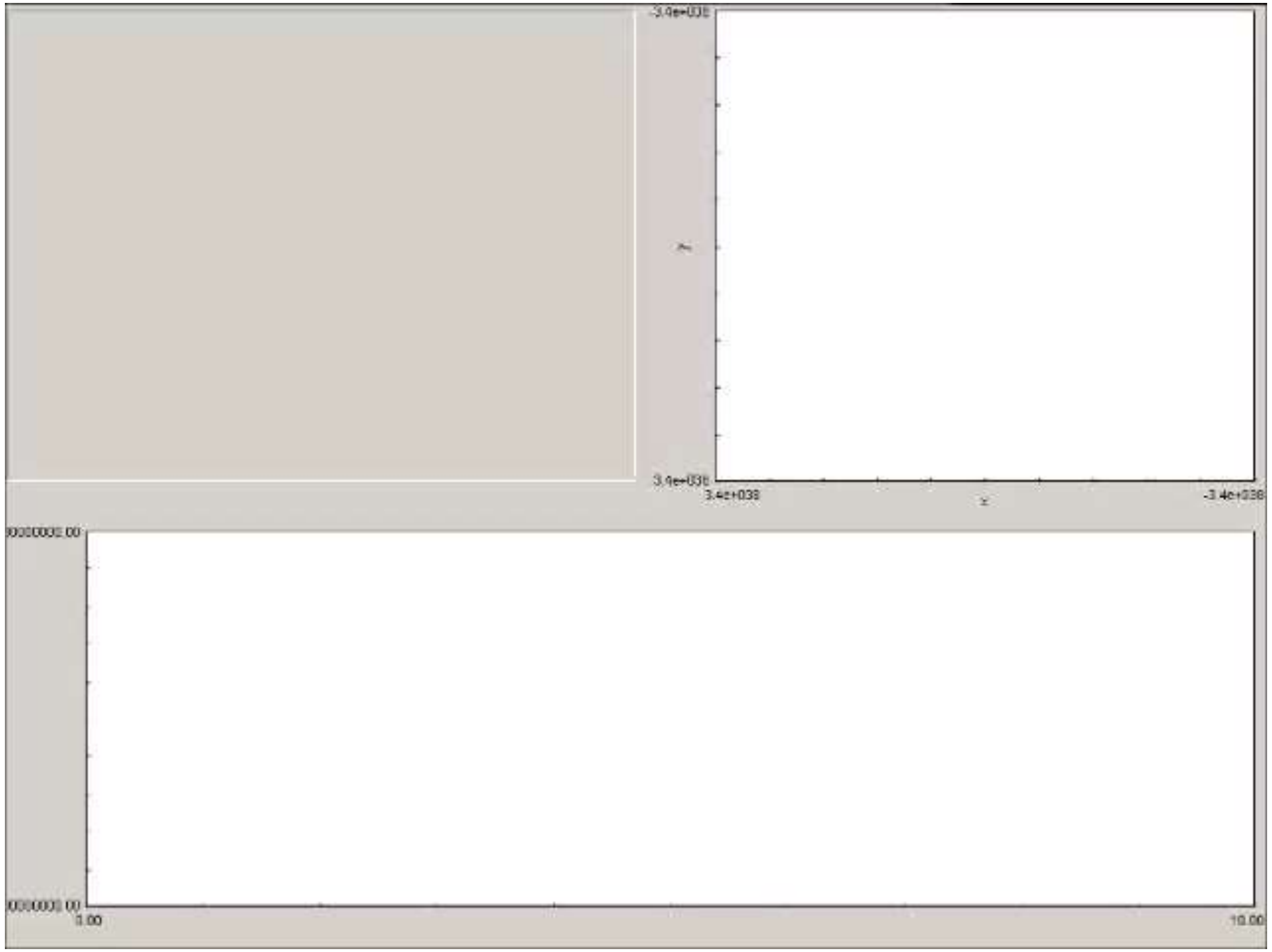
- Coefficients may have different scales and offsets each run



$$\mathbf{H} = \left(\frac{d\theta}{dt}\right)^2 + 2.42847 * \cos(\theta)$$

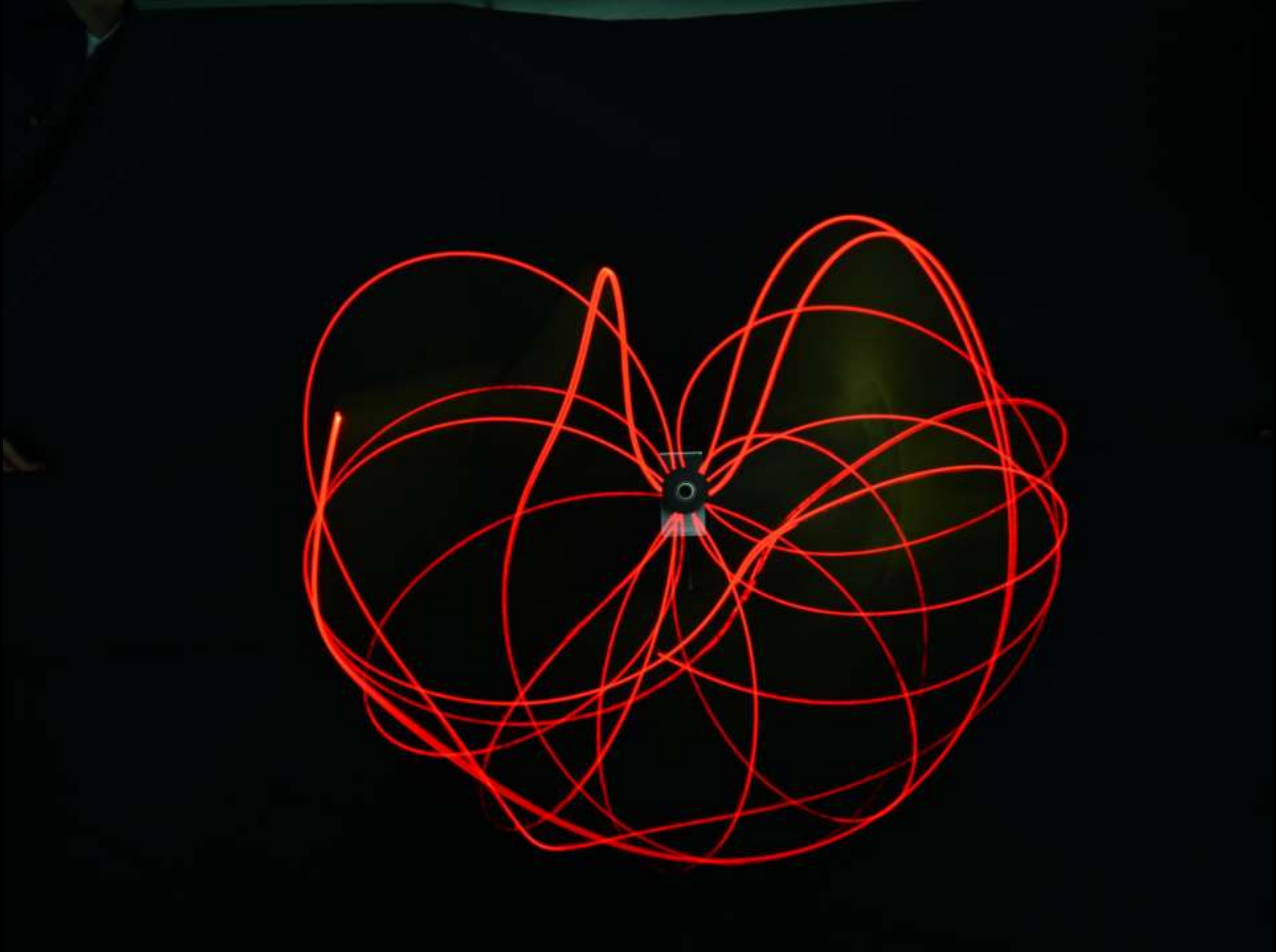
$$\mathbf{L} = 3.52768 * \left(\frac{d\theta}{dt}\right)^2 - 9.43429 * \cos(\theta)$$

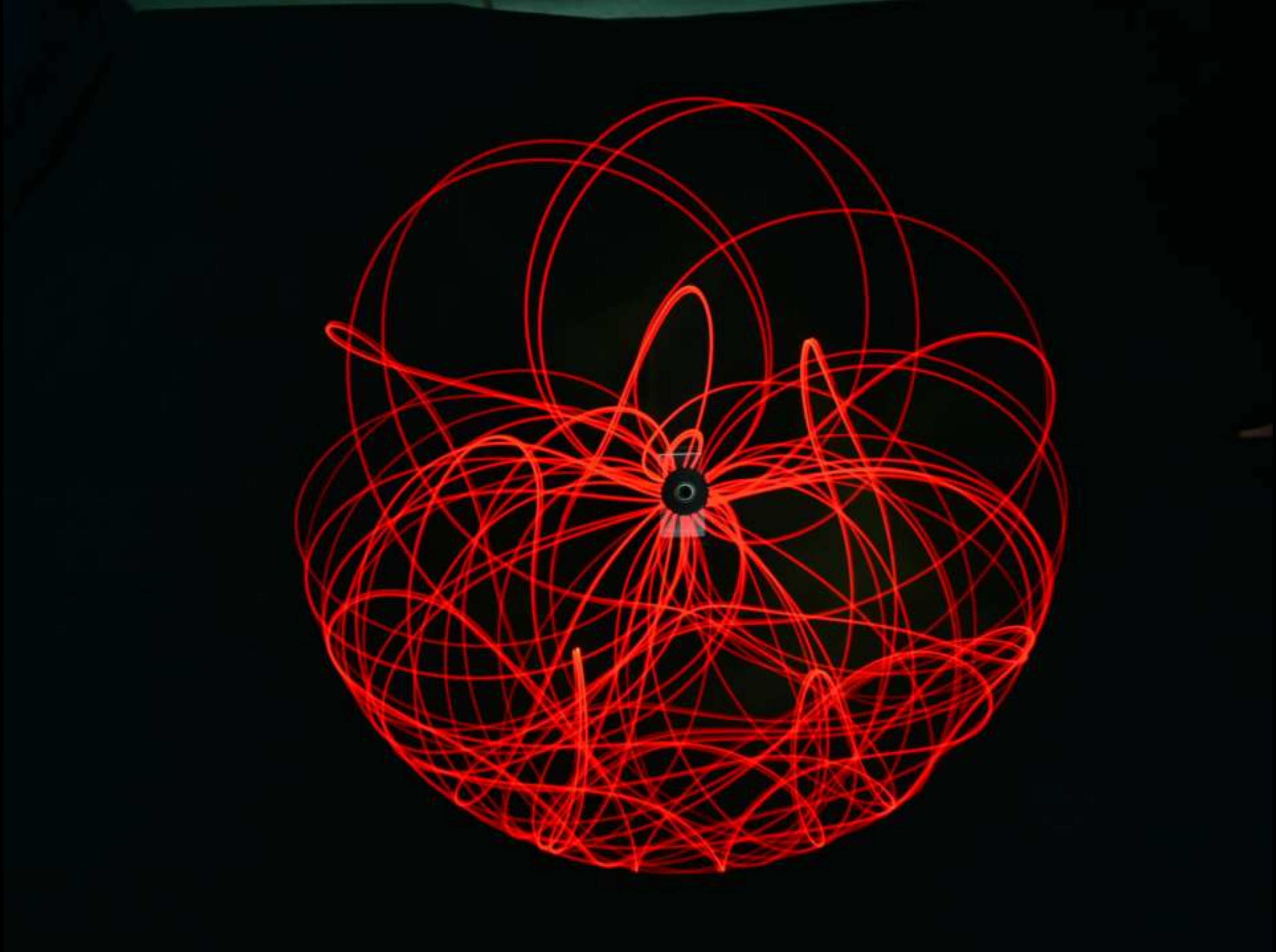
Double Linear Oscillator

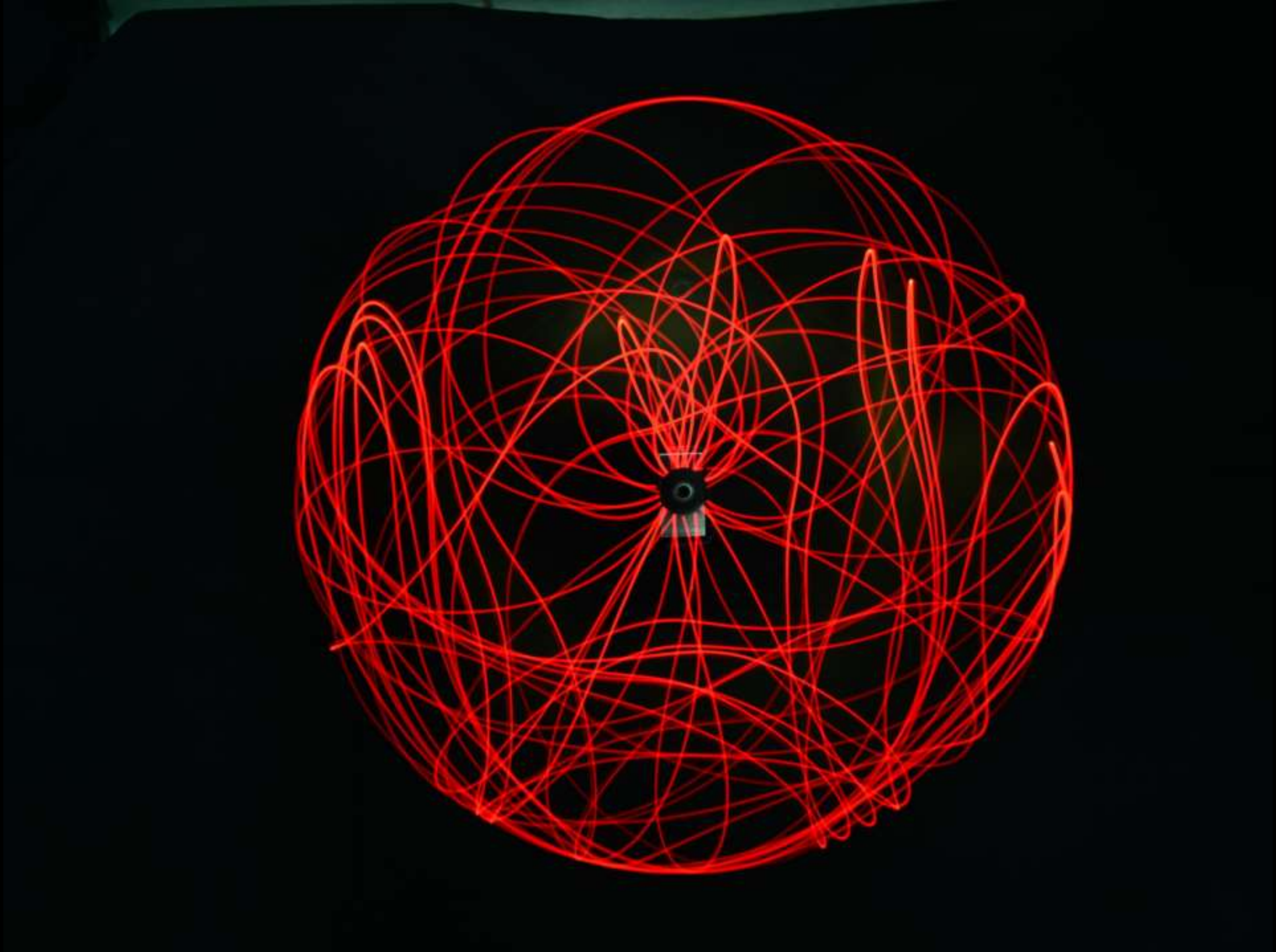


$$\boldsymbol{H} = -14.691 * \boldsymbol{x}_1^2 - 15.551 * \boldsymbol{x}_2^2 - 21.676 * \boldsymbol{x}_1 \boldsymbol{x}_2 + 8.3808 * \left(\frac{\boldsymbol{dx}_2}{\boldsymbol{dt}}\right)^2 + 2.6046 * \left(\frac{\boldsymbol{dx}_1}{\boldsymbol{dt}}\right)^2$$

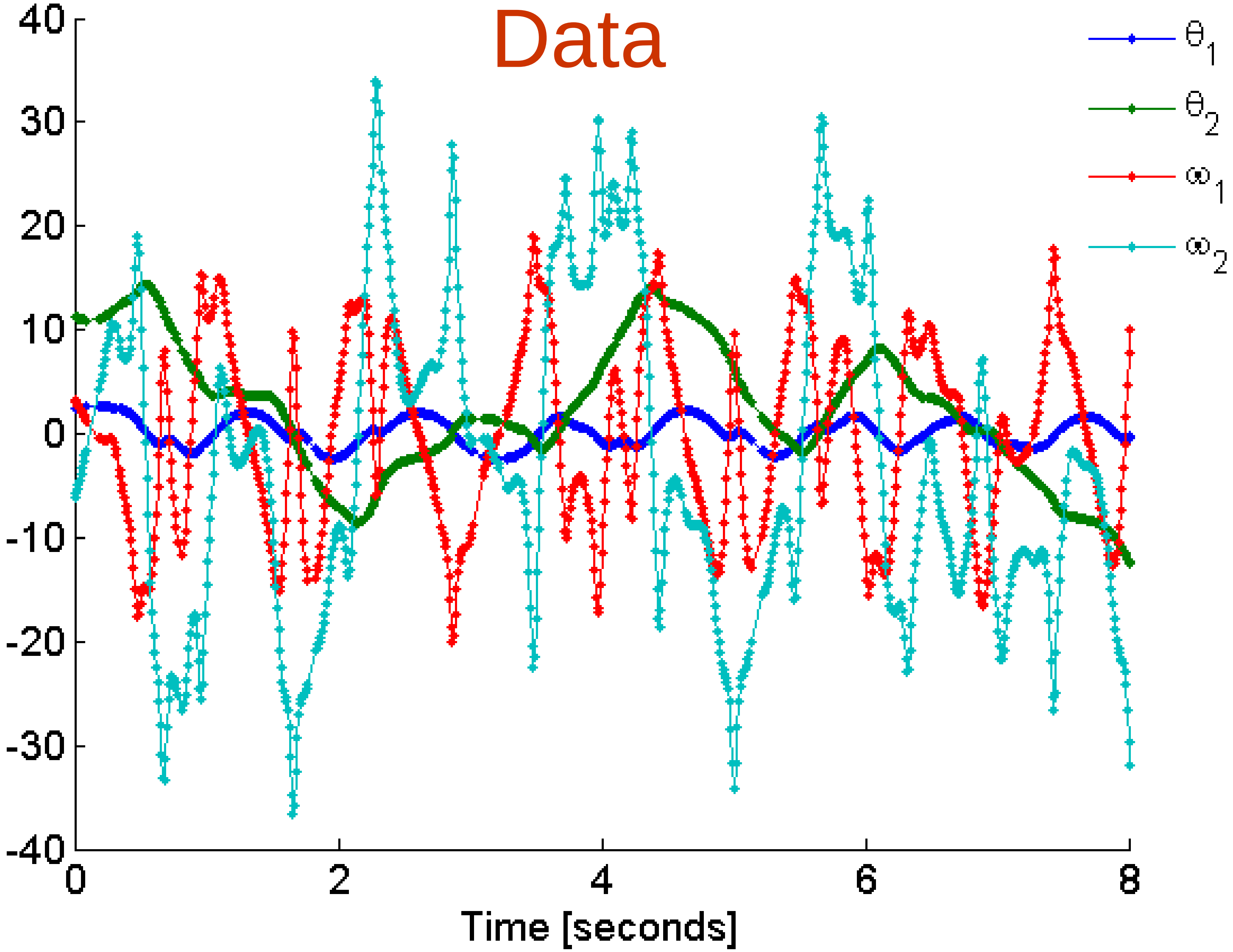
would be plus for Lagrangian

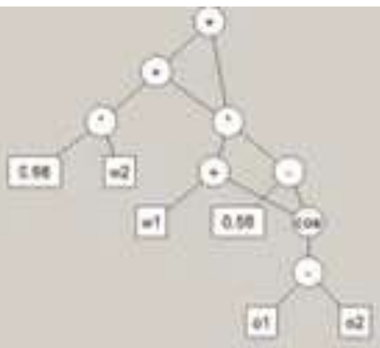




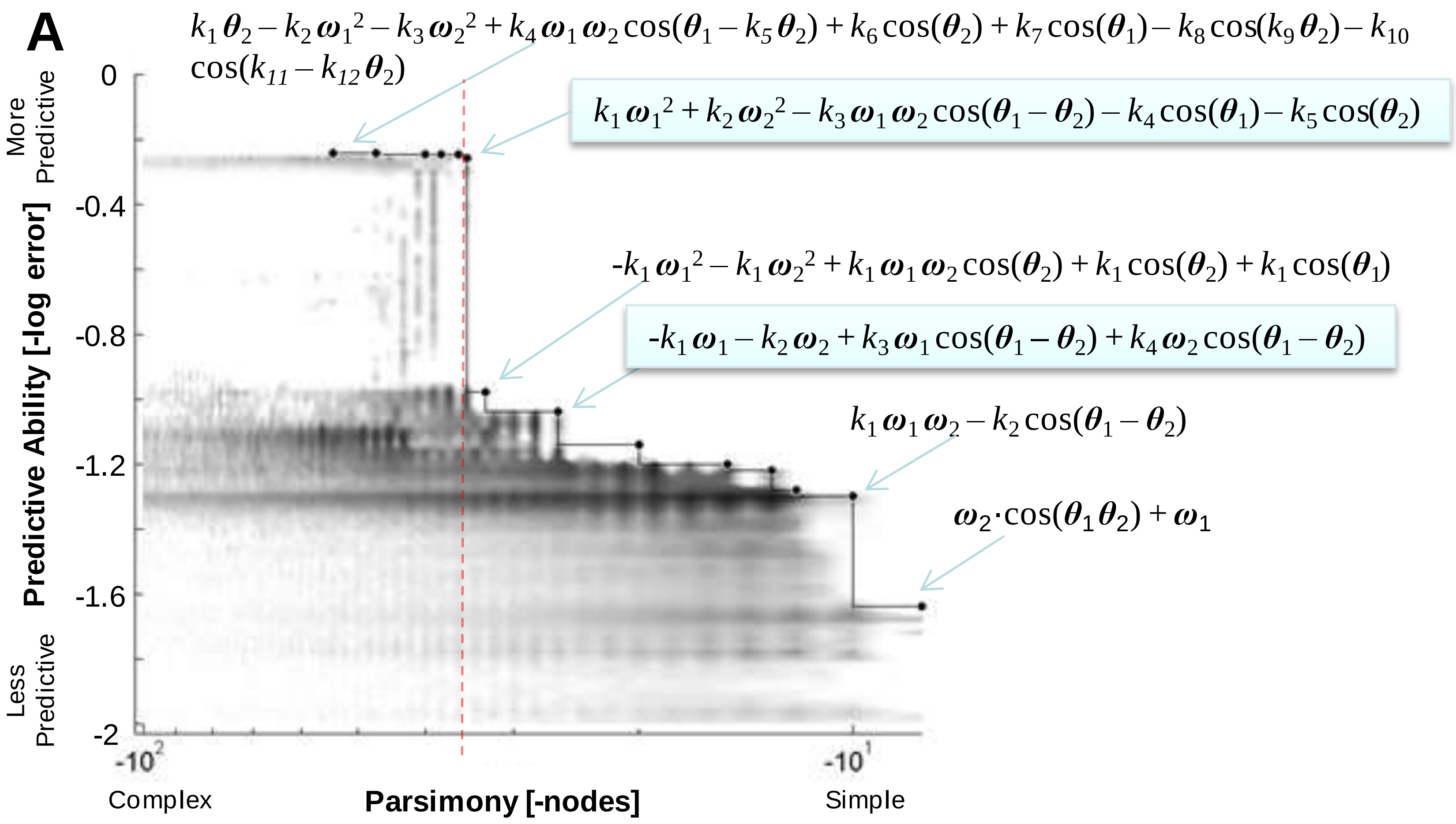


Data

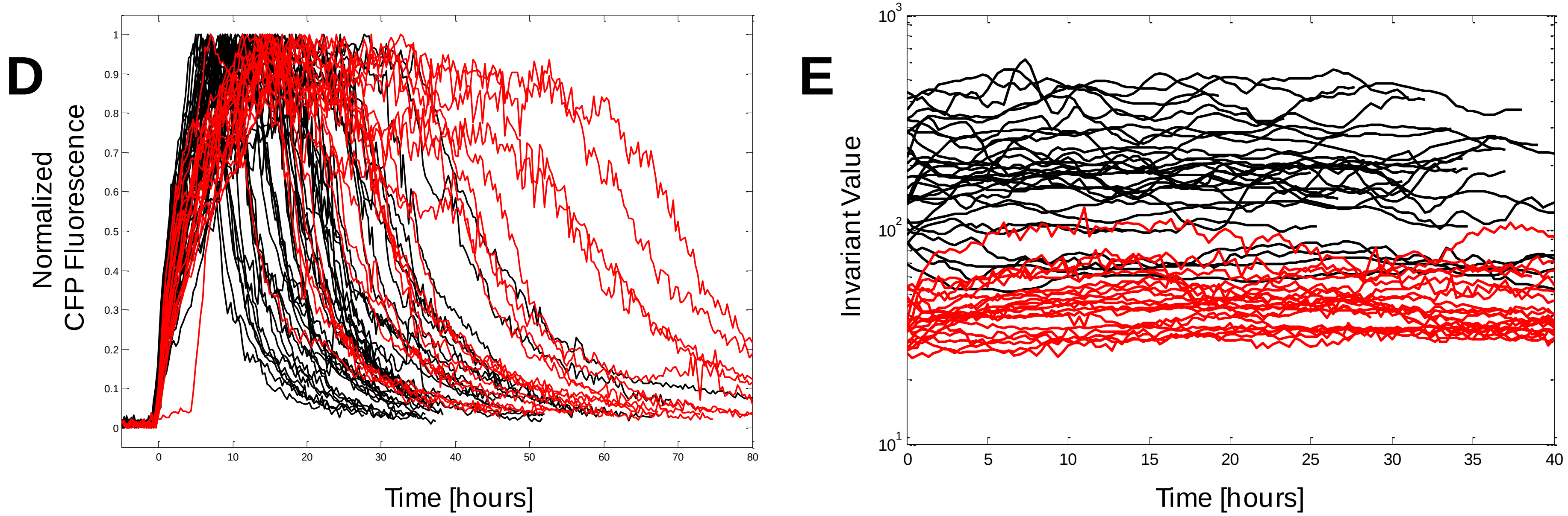


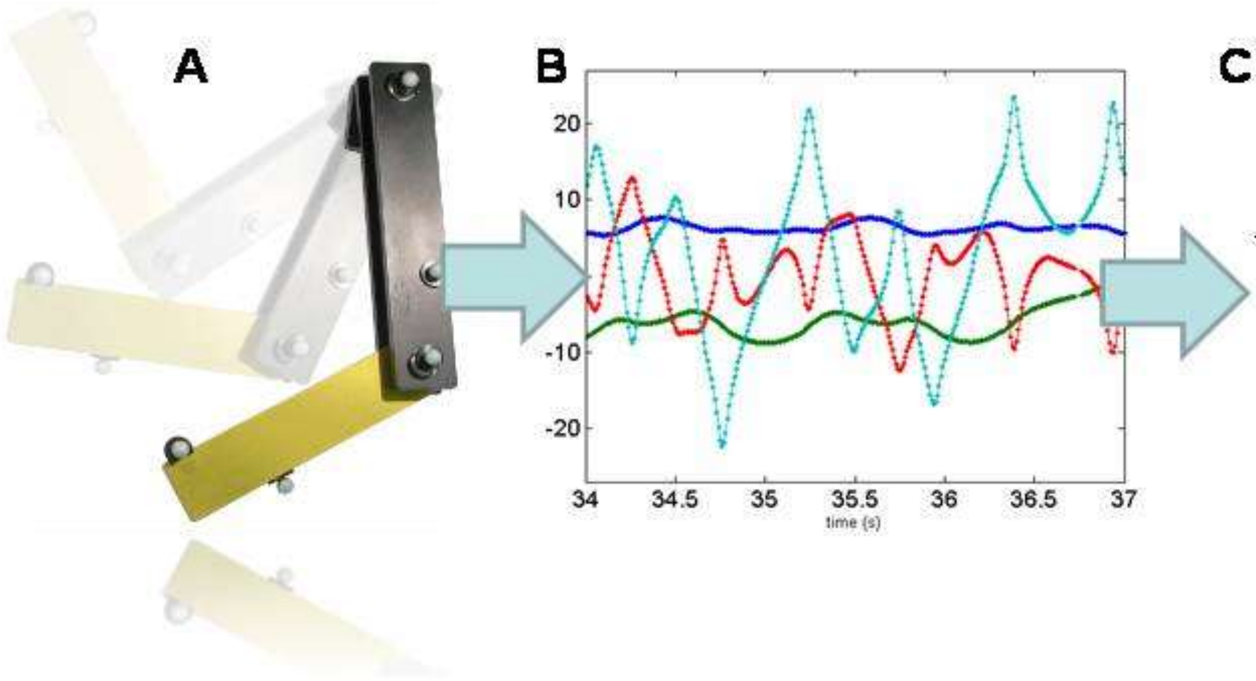


Search for Nontrivial Double Pendulum Law



With Michael D. Schmidt, ***Science***

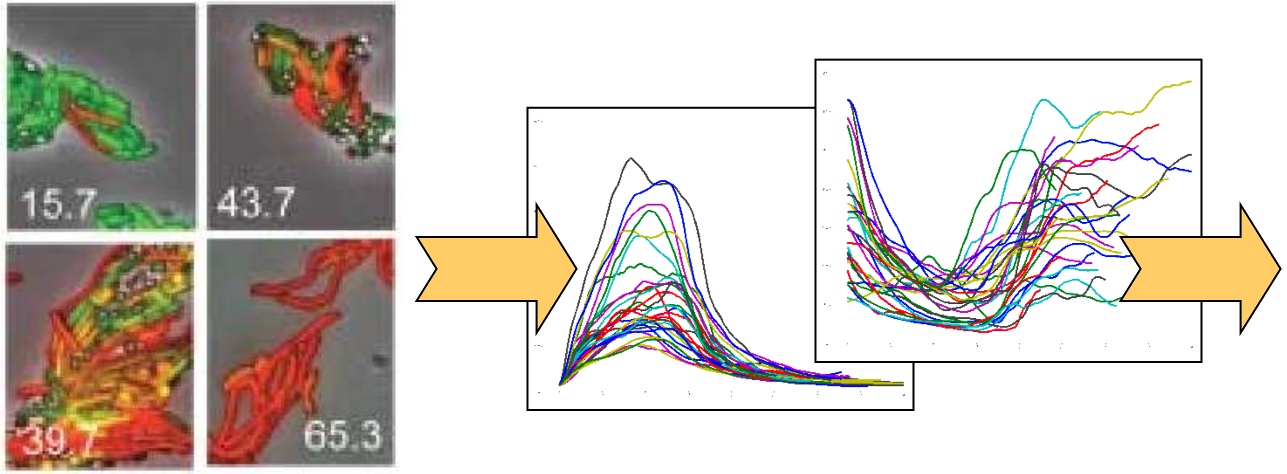

D
Normalized
CFP Fluorescence
Time [hours]
E
Invariant Value
Time [hours]



C

Detected Invariance:

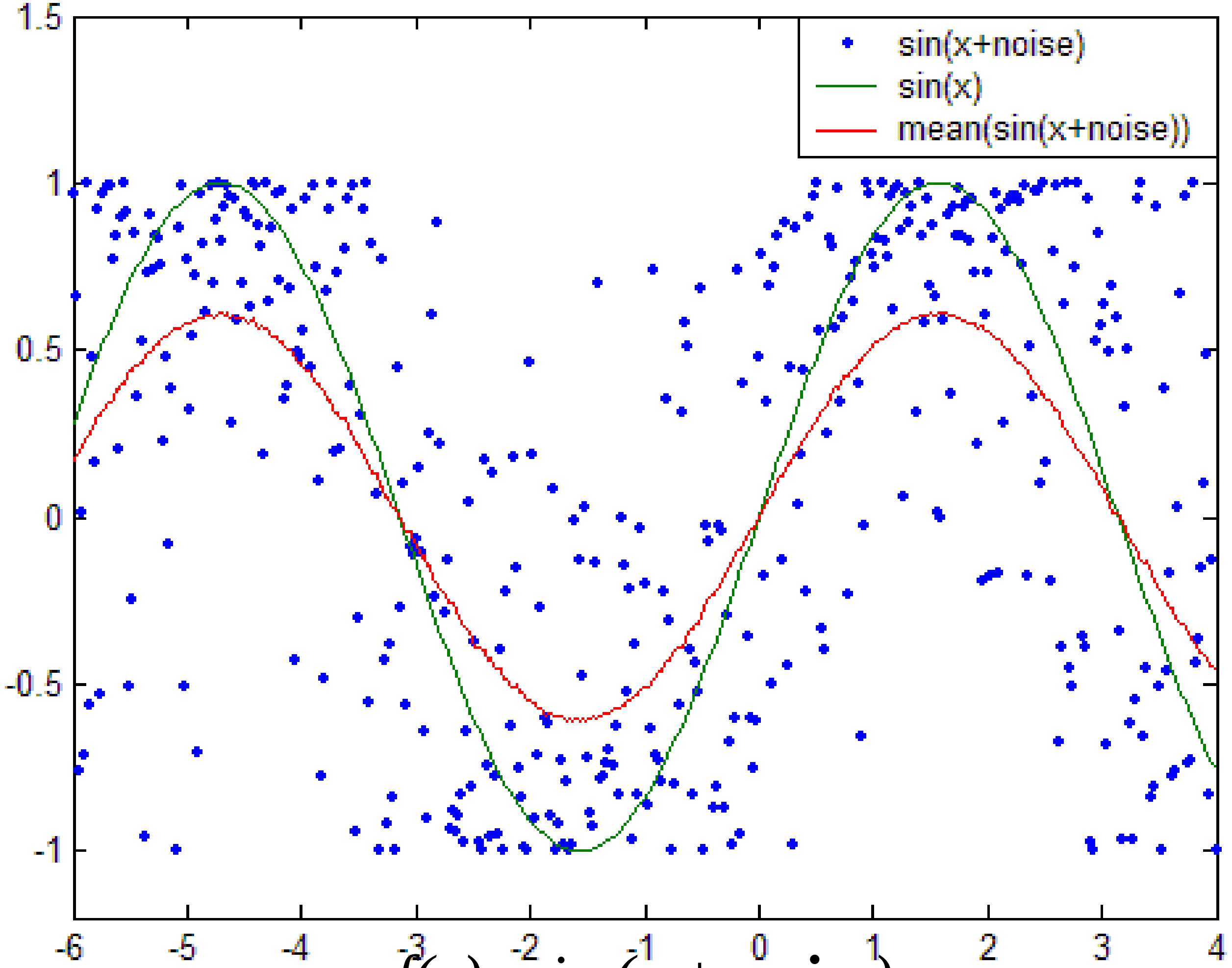
$$L_1^2(m_1+m_2)\omega_1^2 + m_2L_2^2\omega_2^2 + m_2L_1L_2\omega_1\omega_2\cos(\theta_1-\theta_2) - 19.6L_1(m_1+m_2)\cos\theta_1 - 19.6m_2L_2\cos\theta_2$$



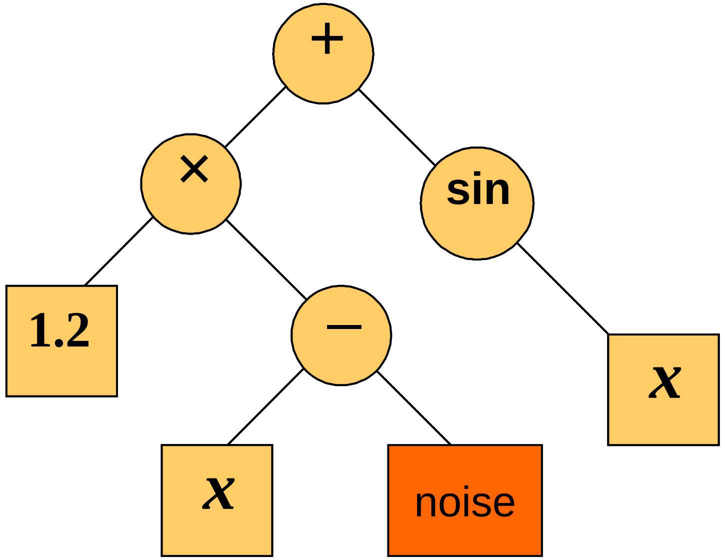
$$\frac{d\boldsymbol{K}}{dt} = a_K + \frac{b_K + c_K\boldsymbol{S}_{t-t_1}}{\boldsymbol{K}_{t-t_2}}$$

$$\frac{d\boldsymbol{S}}{dt} = a_S + \frac{b_S + c_S\boldsymbol{K}_{t-t_3}}{\boldsymbol{S}_{t-t_4}}$$

Stochastic Models

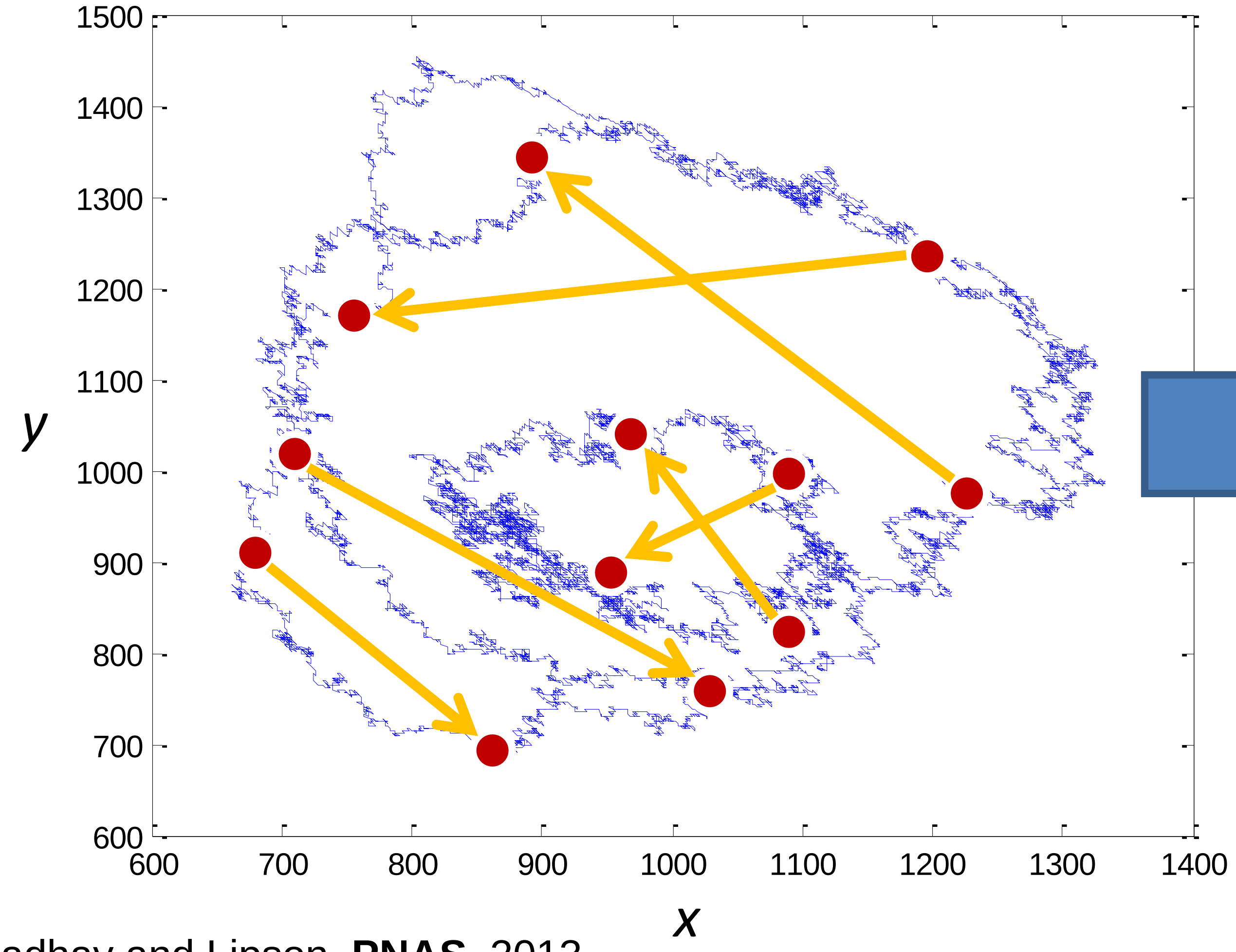


$f(x)=\sin(x + \boldsymbol{noise})$



Reaction Systems

Periodic Samples of a Stochastic System



Maximum Likelihood Stochastic Model

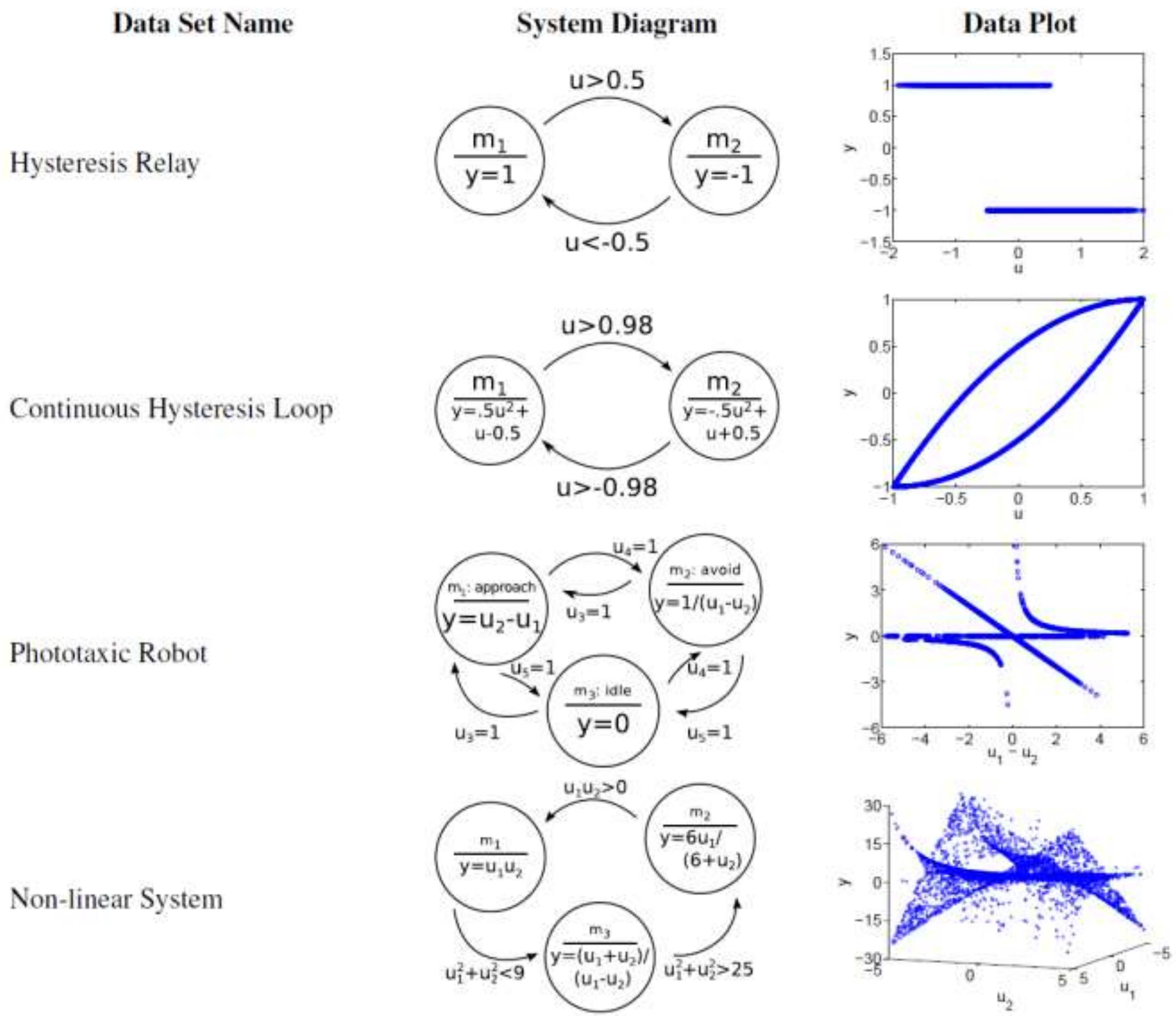
$$x \xrightarrow{10} 2x$$

$$x + y \xrightarrow{0.1} 2y$$

$$y \xrightarrow{10} \varnothing$$

Chattopadhay and Lipson, **PNAS**, 2013

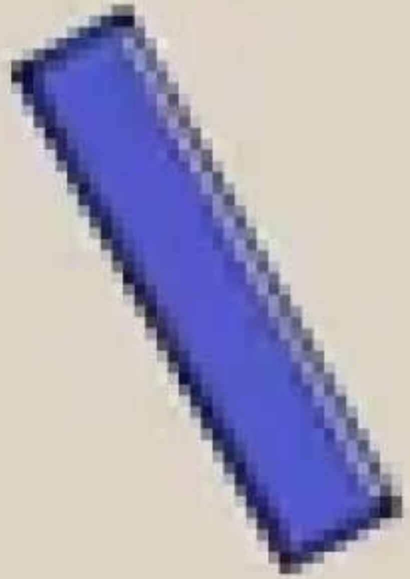
Hybrid Systems



Daniel Ly, Learning Symbolic Representations of Hybrid Dynamical Systems

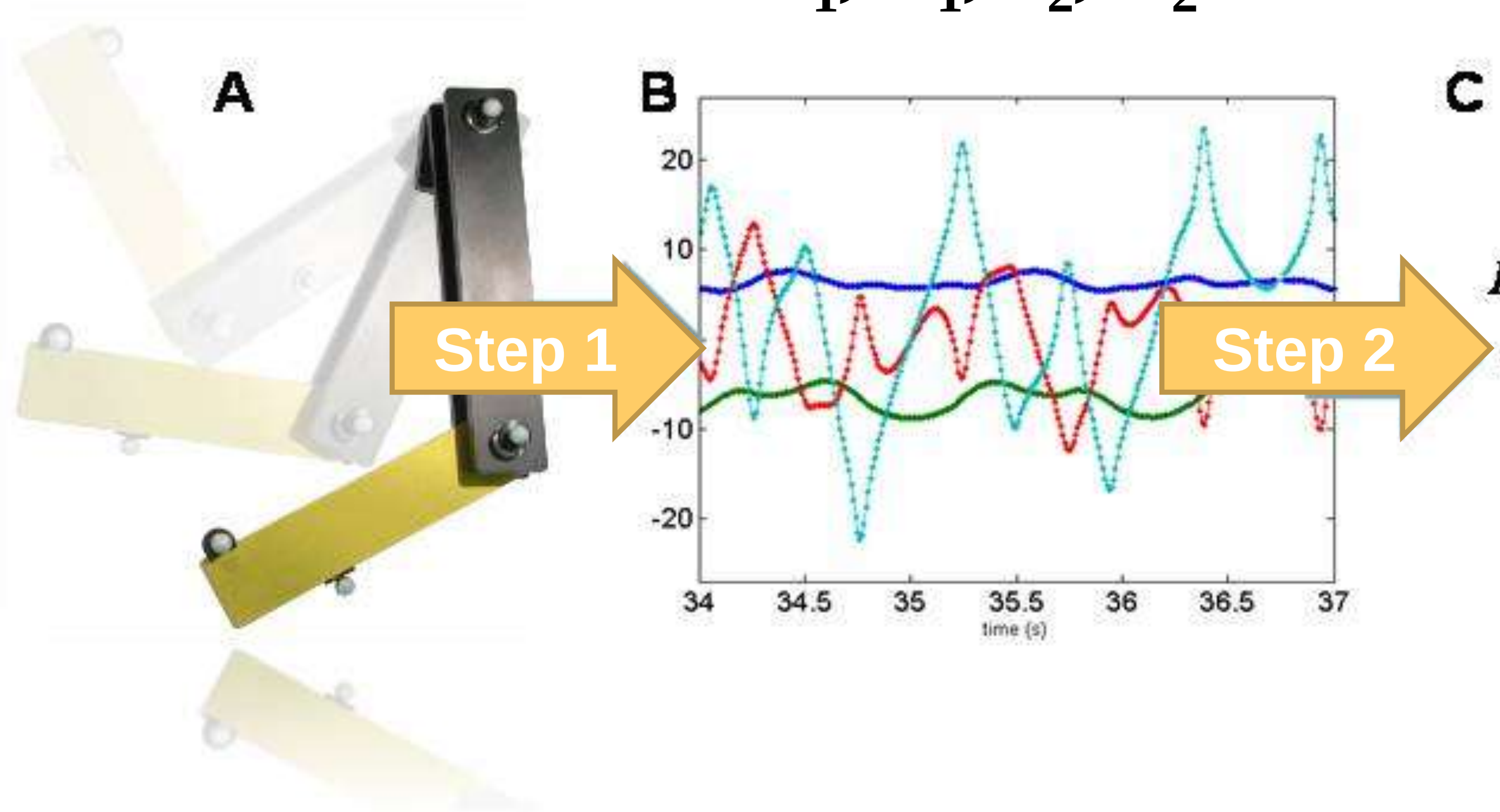
With Daniel Ly

$$\theta_t \, , \, \omega_t$$



$$f(\theta_t, \, \omega_t) = const$$

$\theta_1, \omega_1, \theta_2, \omega_2$



C

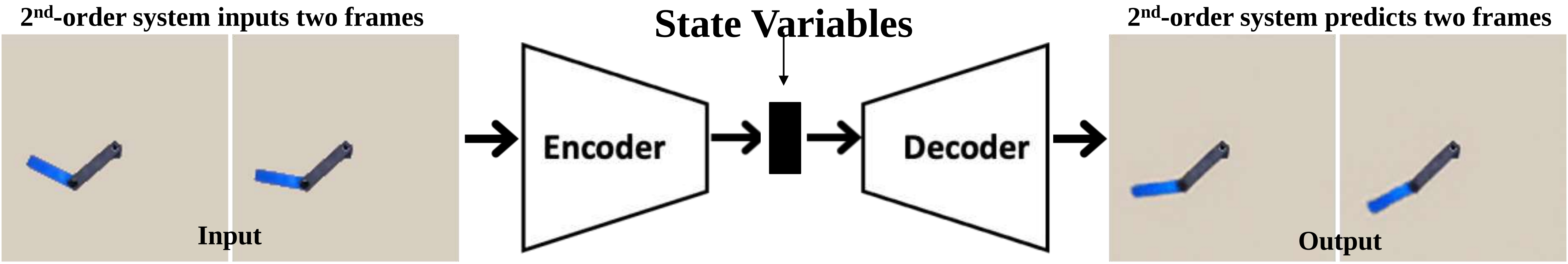
Detected Invariance:

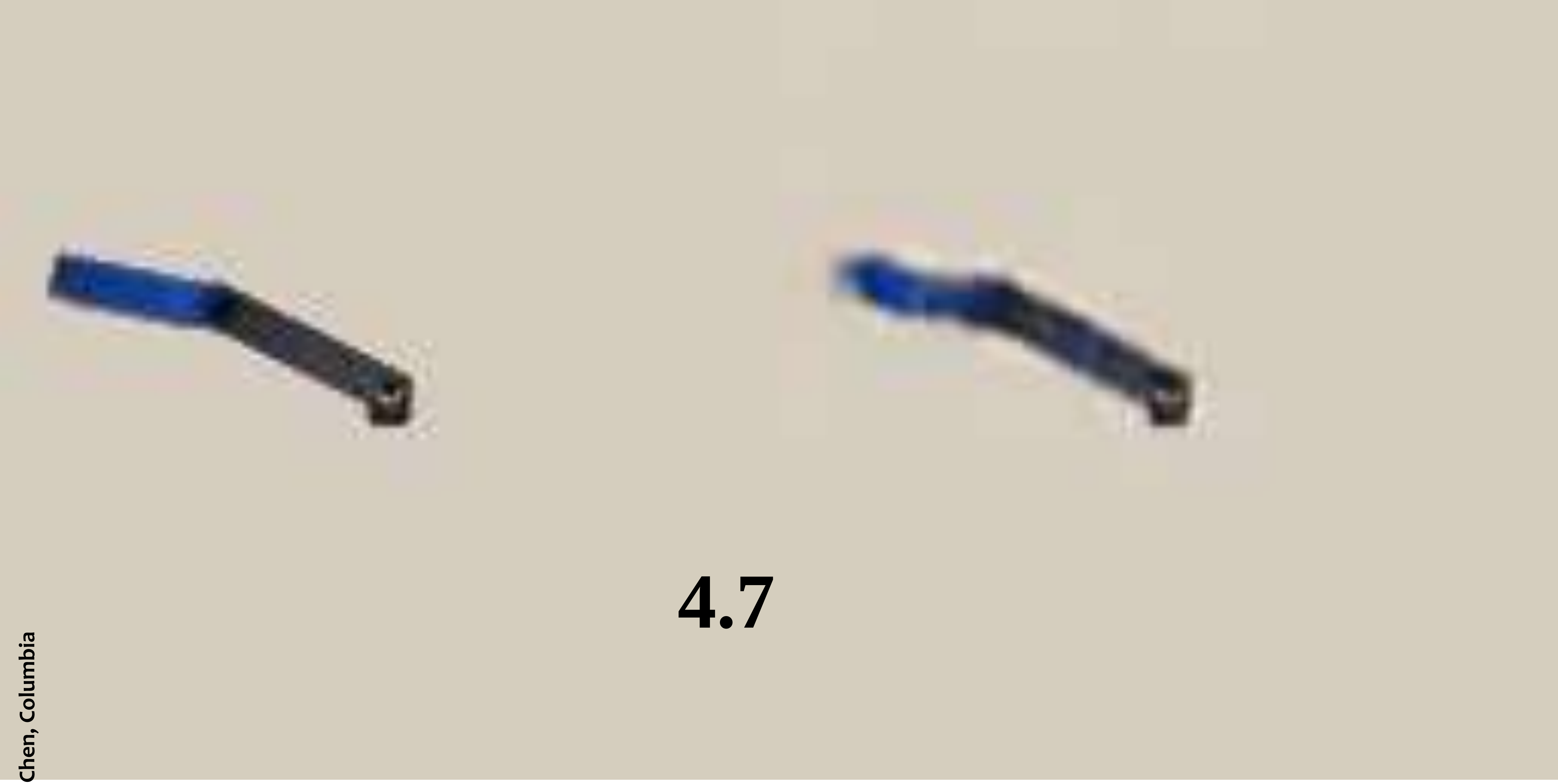
$$L_1^2(m_1+m_2)\omega_1^2 + m_2L_2^2\omega_2^2 + m_2L_1L_2\omega_1\omega_2\cos(\theta_1 - \theta_2) - 19.6L_1(m_1+m_2)\cos\theta_1 - 19.6m_2L_2\cos\theta_2$$

Boyuan Chen, Columbia

Real **Predicted**

(~0.5 sec in advance)


2nd-order system inputs two frames
State Variables
2nd-order system predicts two frames
Encoder
Decoder
Input
Output



Real

Predicted
(~0.5 sec in advance)

Boyuan Chen, Columbia

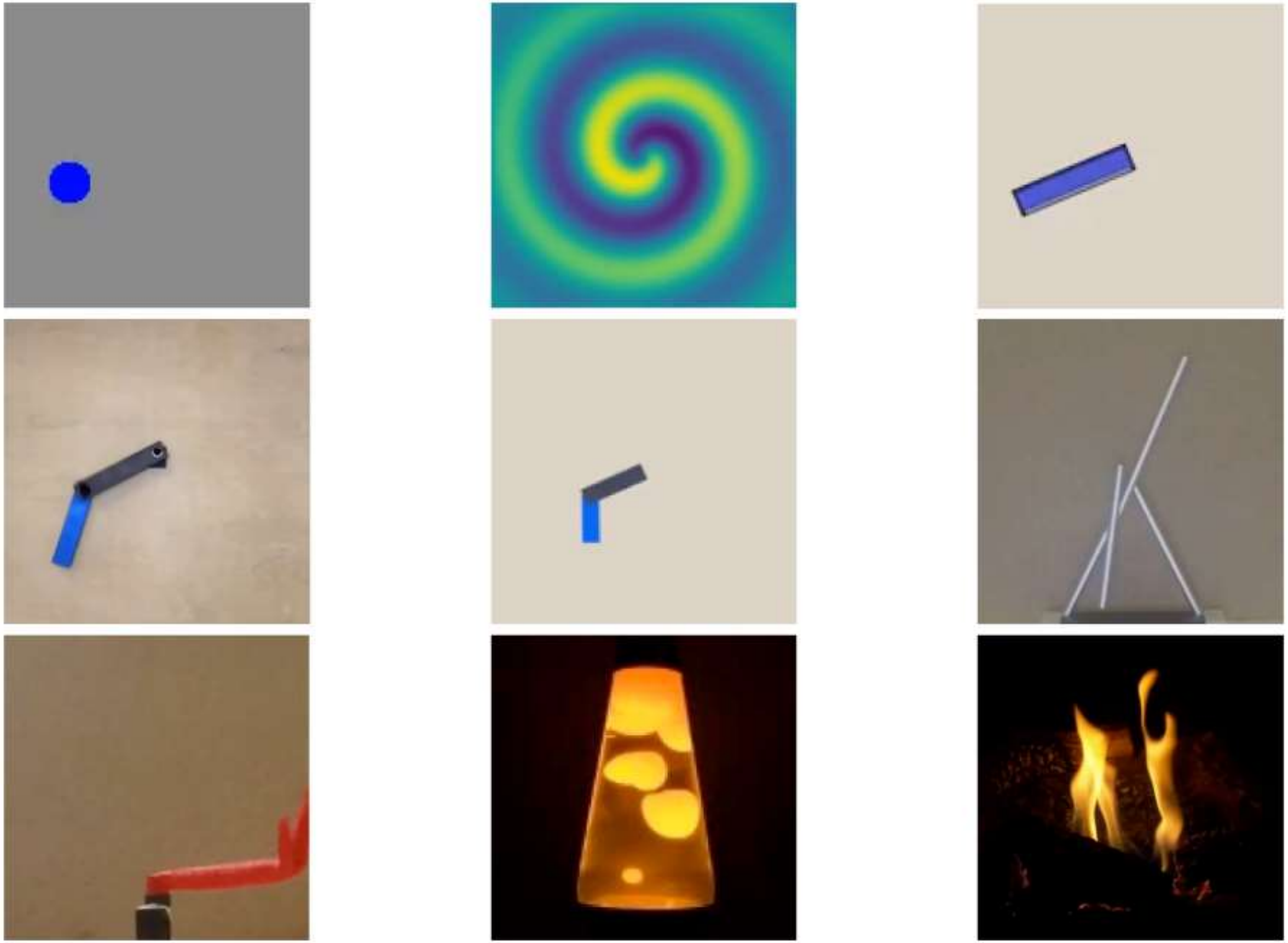
Real

24

Predicted

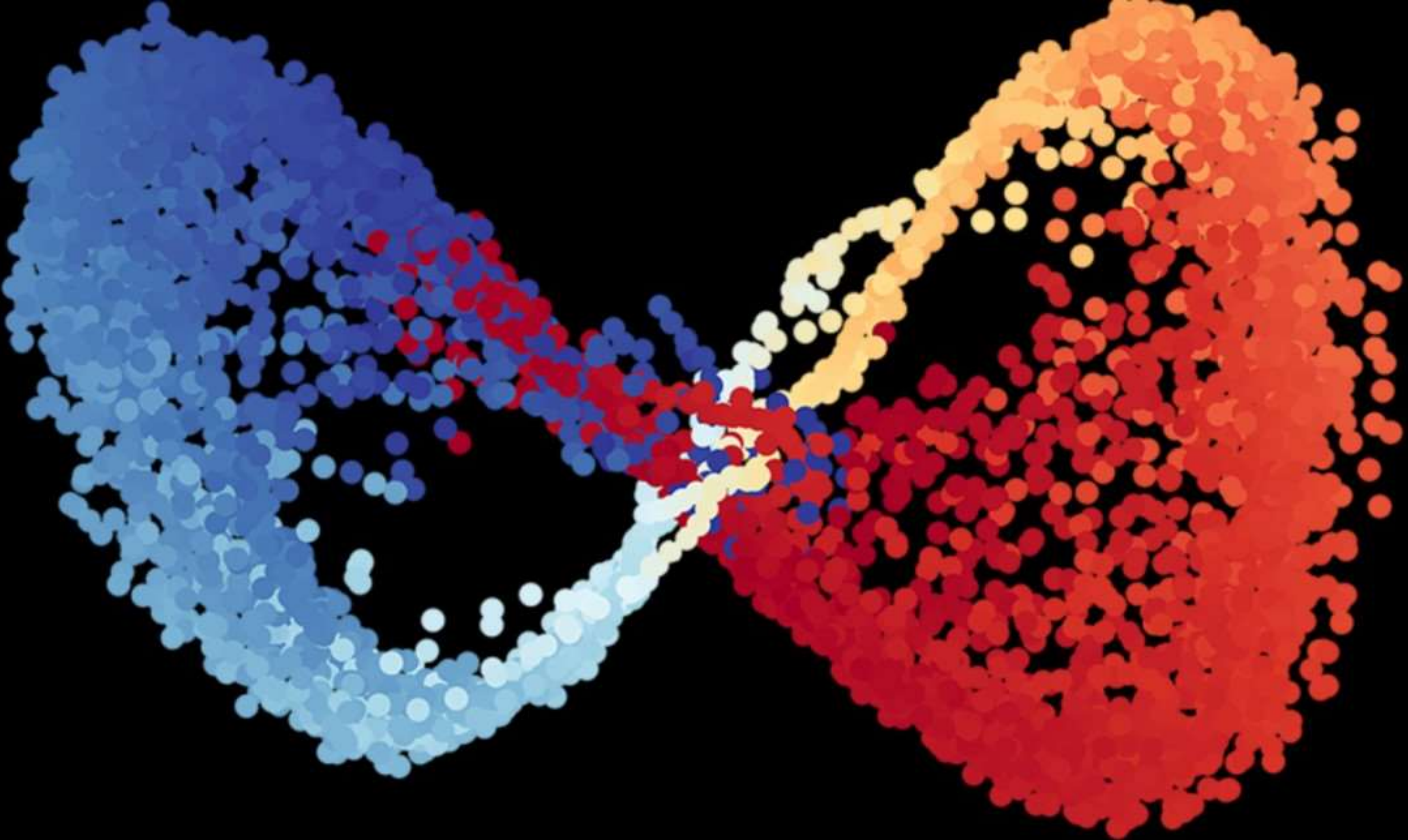
(~0.5 sec in advance)

Boyuan Chen, Columbia



Chen, Huang, Raghupathi, Preetam, Du, Lipson. In review. 2022

System	ID from Latent Vectors	Ground Truth
Circular motion	2.19 (± 0.05)	2
Reaction diffusion	2.16 (± 0.14)	2
Single pendulum	2.05 (± 0.02)	2
Rigid double pendulum	4.71 (±0.03)	4
Swing stick	4.89 (± 0.33)	4
Elastic double pendulum	5.34 (± 0.20)	6
Air dancer	7.57 (± 0.13)	Unknown
Lava lamp	7.89 (±0.96)	Unknown
Fire	24.70 (± 2.02)	Unknown



$$f=ma$$

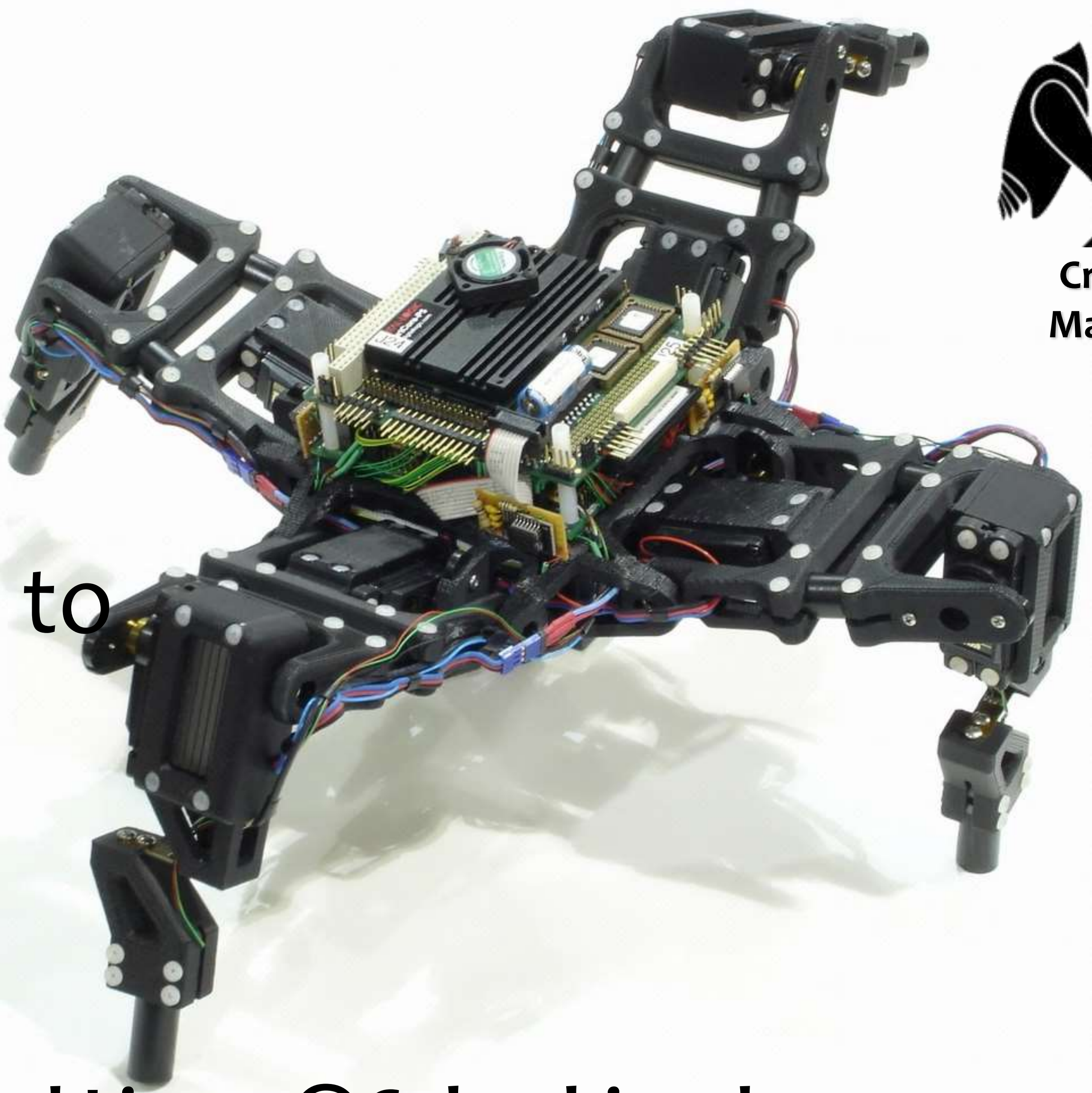
1687

The New York Times

"… Theoretical physicists are not yet obsolete, but scientists have taken steps toward replacing themselves …"

The AI Scientist

Automating discovery, from cognitive robotics to computational biology



Creative Machines Lab

For copy of slides email **Hod.Lipson@Columbia.edu**

This research was supported in part by