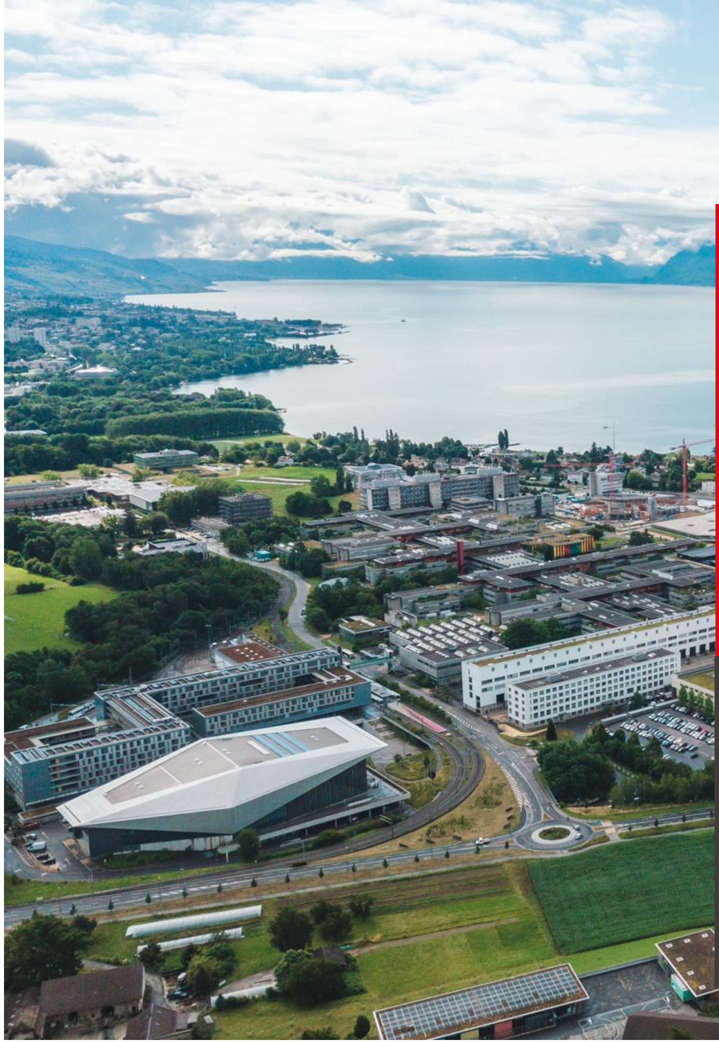


Graph Neural Network with a Physics Inductive Bias for Multi-body Dynamical System

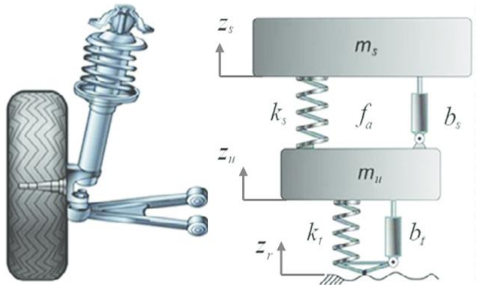
Vinay Sharma, Olga Fink

Intelligent Maintenance and Operations System, EPFL

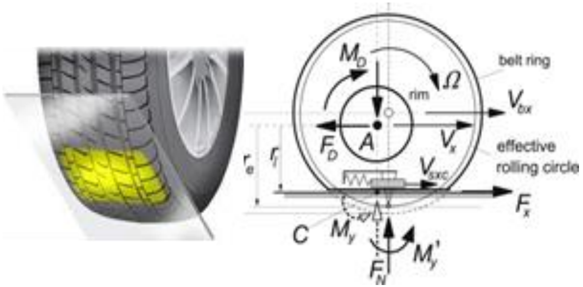
04 September 2024

École polytechnique fédérale de Lausanne

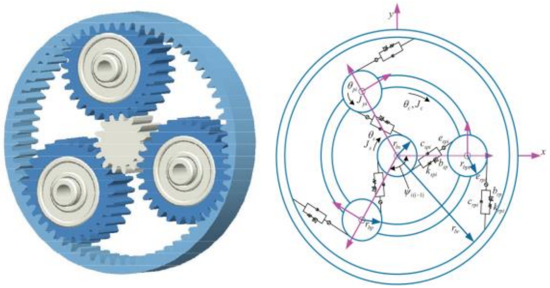
Multi-Body Dynamical Systems:
Integral to Industrial Applications



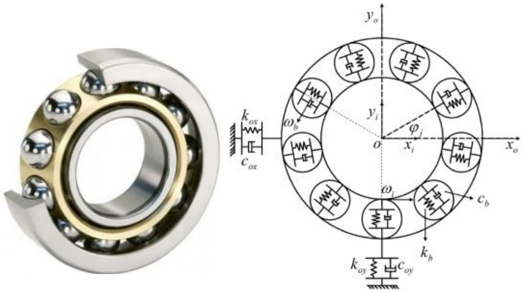
Suspension Systems



Tire-road Contact

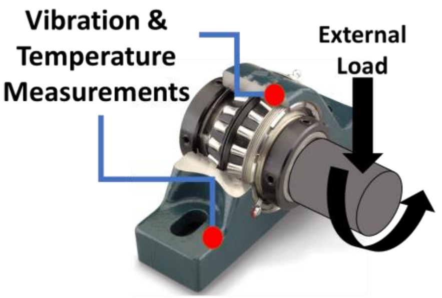


Planetary Gears



Roller Bearings

Motivation : Need for Dynamical Models



Operational & Condition Monitored Bearing

Crack Propagation (Paris Law) : $\frac{da}{dN} = m\Delta K^b$

Creep Damage Model : creep rate = $AT^n\sigma^m$

Wear Damage Model: Wear rate = $V_{wear} = K\left(\frac{WL}{3H}\right)$

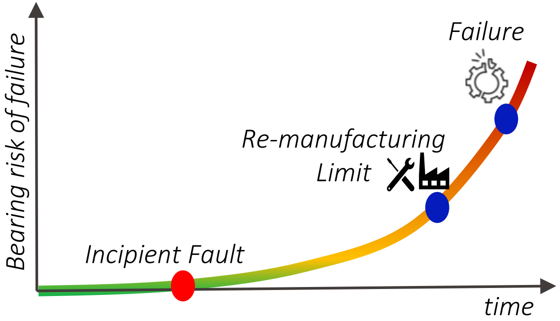
Damage Models

Stress Intensity Factor at Crack Tip

Contact Stresses

Contact Loads

Internal Loads that can not be measured !

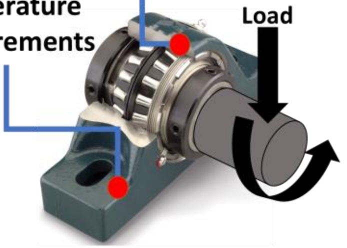


Early Diagnostics & Long Range Prognostics

Motivation : Need for Dynamical Models

Vibration & Temperature Measurements

External Load



Operational & Condition Monitored Bearing

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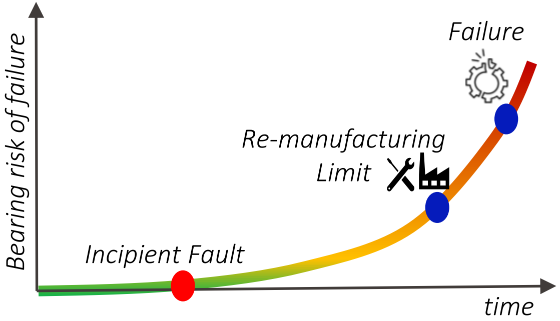
Damage Models



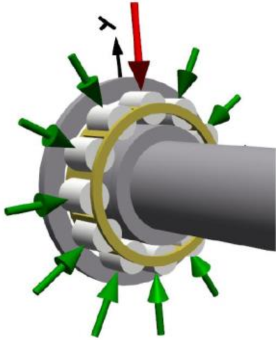
Early Diagnostics & Long Range Prognostics

Stress Intensity Factor at Crack Tip

Contact Stresses

Contact Loads

Dynamical Models Transform the Operating Conditions & Measurements to Internal Loads



Attributes of an Ideal Dynamics Model

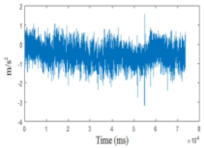
OUTPUT

On-line Dynamics Prediction as a function of Changing Operating Conditions.

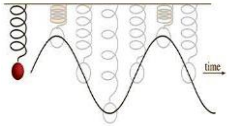
Interpretable & Explainable dynamics

Long trajectory roll-out & stable error accumulation

INPUT DATA

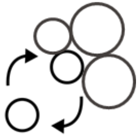


Noisy input data

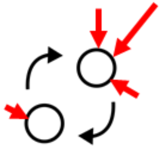


Learning from trajectory without parameters as input

GENERALIZATION

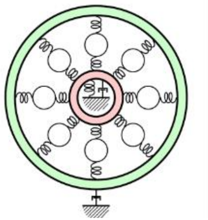


Extrapolation to Unseen Configurations

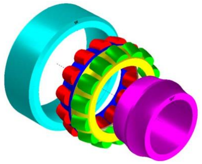


Generalization to unseen operating conditions

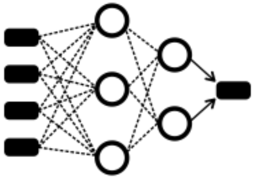
Traditional Approaches to Model Dynamics



Lumped Parameter Models



FEA/Multiphysics Simulations



Data Driven Methods Feed Forward Neural Networks, PINNS

Li & Lee (2005).
Gear fatigue crack prognosis using embedded model, gear dynamic model and fracture mechanics. *Mechanical systems and signal processing*

Developed a **dynamic model** of a **gear transmission** to estimate the **internal loads** from **measurements** for **RUL prediction using Paris Law**

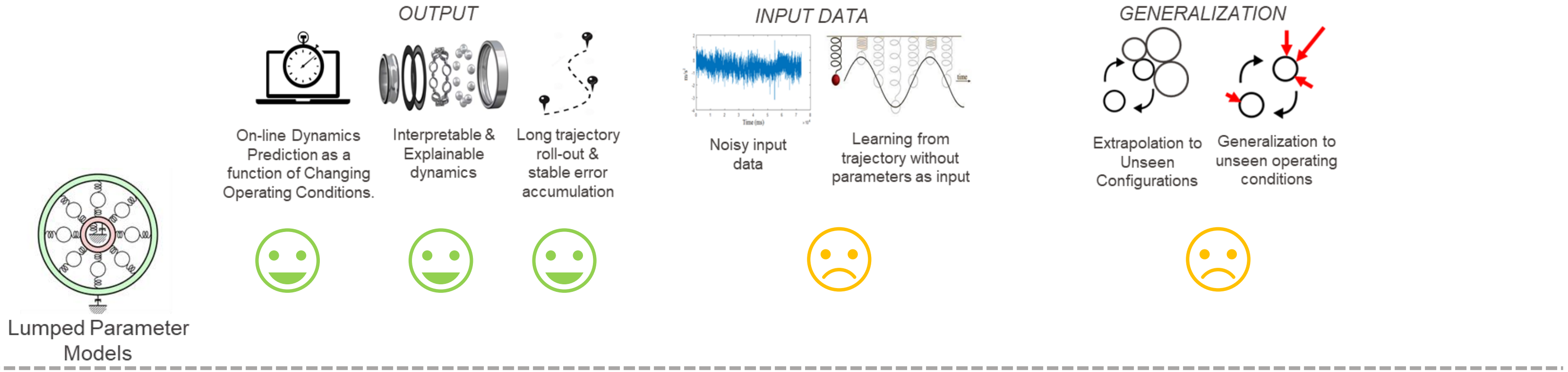
Kacprzynski, et. al. (2002).
Enhancement of physics-of-failure prognostic models with system level features.
IEEE aerospace conference

Combination of **Paris law** along with a simplified two-dimensional (2D) **FEA** for **estimating stress-intensity-factor** RUL estimation of Helicopter Gears

Pavlenko, et.al. (2019).
Application of artificial neural network for identification of bearing stiffness characteristics in rotor dynamics analysis.
International Conference on Design, Simulation, Manufacturing, 2018

ANN trained on **FEA model** data to predict **bearing stiffness** as a function of rotor speed.

Traditional Approaches to Model Dynamics



- Hu, Y., Miao, X., Si, Y., Pan, E., & Zio, E. (2022). Prognostics and health management: A review from the perspectives of design, development and decision. *Reliability Engineering & System Safety*, 2022
- Thelen, A., Zhang, X., Fink, O., Lu, Y., Ghosh, S., Youn, B.D., Todd, M.D., Mahadevan, S., Hu, C. and Hu, Z., 2022. A comprehensive review of digital twin—part 1: modeling and twinning enabling technologies. *Structural and Multidisciplinary Optimization, 2022*

Traditional Approaches to Model Dynamics

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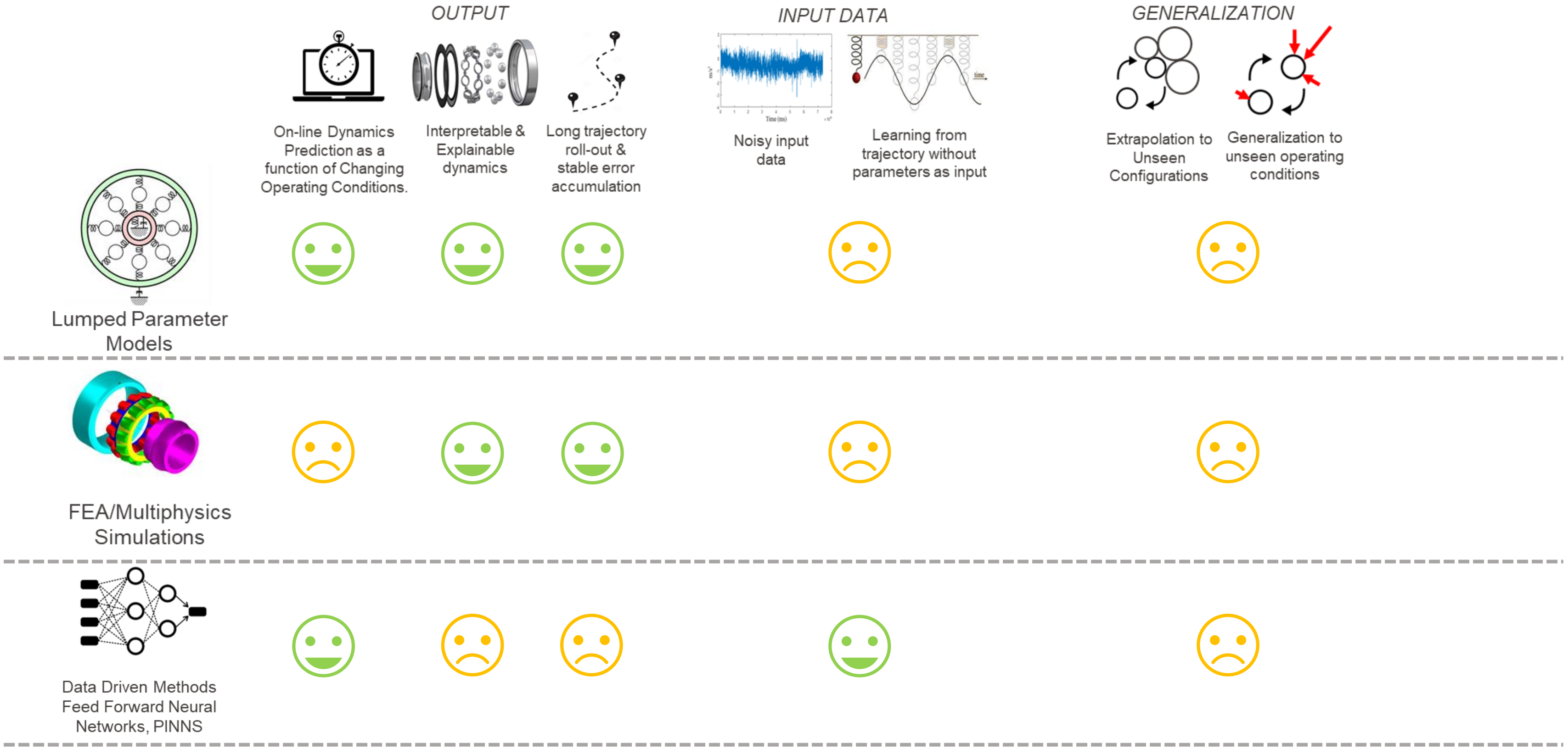
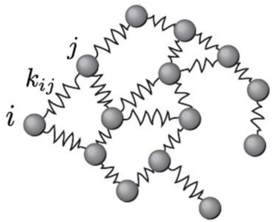
Traditional Approaches to Model Dynamics



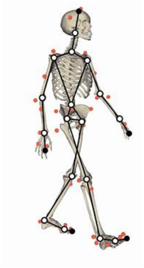
- Hu, Y., Miao, X., Si, Y., Pan, E., & Zio, E. (2022). Prognostics and health management: A review from the perspectives of design, development and decision. *Reliability Engineering & System Safety*, 2022
- Thelen, A., Zhang, X., Fink, O., Lu, Y., Ghosh, S., Youn, B.D., Todd, M.D., Mahadevan, S., Hu, C. and Hu, Z., 2022. A comprehensive review of digital twin—part 1: modeling and twinning enabling technologies. *Structural and Multidisciplinary Optimization, 2022*

Recent Progress:
Graph Neural Network Based Approaches for Learning Dynamics

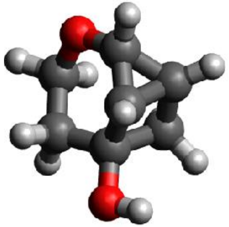
GNNs excel at modelling systems driven by pair-wise interactions



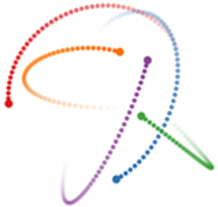
Spring-Mass Systems



Motion Dynamics

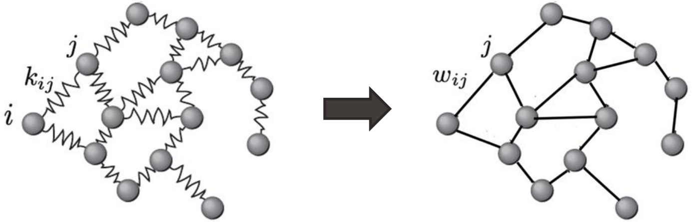


Molecular Dynamics



Particle Dynamics

GNNs Incorporate Spatial Inductive Bias :



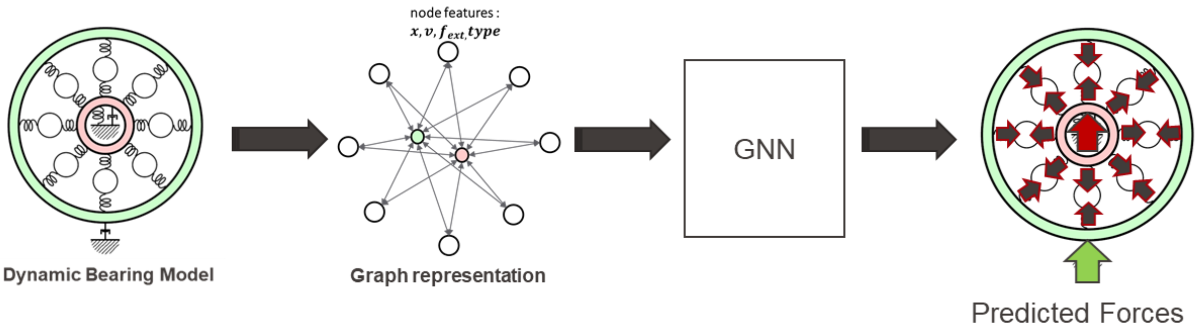
Spatial Connectivity Between Different Components is explicitly modelled

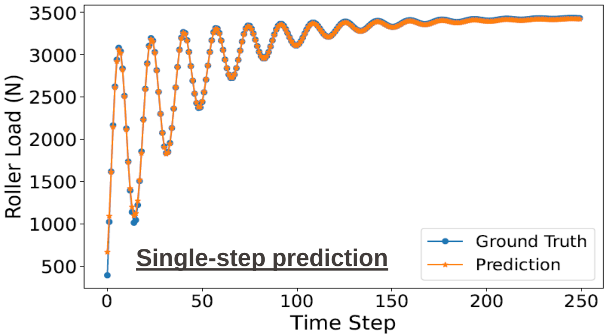
- Zhou, Jie, et al. "Graph neural networks: A review of methods and applications." *AI open 1,* 2020
- Sanchez-Gonzalez, Alvaro, et al. "Learning to simulate complex physics with graph networks." *International conference on machine learning*. PMLR, 2020.

Recent Progress:

E.g. Graph neural networks for dynamic modeling of roller bearings

Sharma, V., Ravesloot, J., Taal, C., & Fink, O. , Annual Conference of the PHM Society, 2023





Inspired by Lumped Parameter Models Graph Representations of Multi-Body Industrial Systems are straightforward.

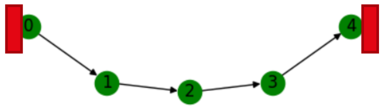
GNN based Dynamics Model:
Details of Data-Driven Interaction Learning

State of the art method:

Graph Neural Simulator,

Learning to simulate complex physics with graph networks." Sanchez-Gonzalez, et.al., ICML 2020

How GNNs Model Dynamics? : Example of a Spring-Mass dynamical System:

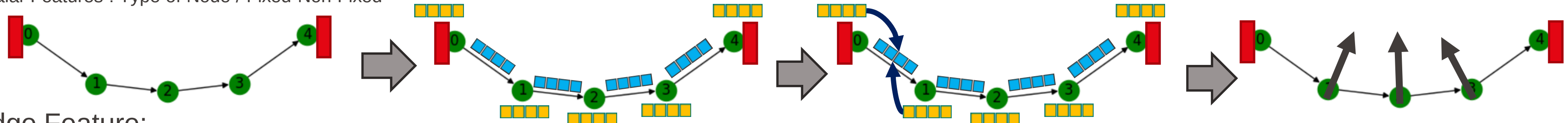


The Dynamical System is Represented as a Graph where:
- Each Node represent the mass
- Each Edge represent the spring

Node Feature:

Dynamics Features : Position, Velocity

Scalar Features : Type of Node / Fixed-Non Fixed



Edge Feature:

Dynamics Features : Relative distance between Nodes

Scalar Feature : Type of Edge (e.g. Damper/Spring)

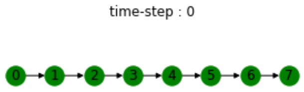
Encode:
Transform Features to N dimensional Numerical Representation

Process:
Transform Node and Edge Representations by Adding neighbouring node representation.

Decode:
Node Representations are decoded as Node accelerations

GNN based Dynamics Model:
Details of Data-Driven Interaction Learning

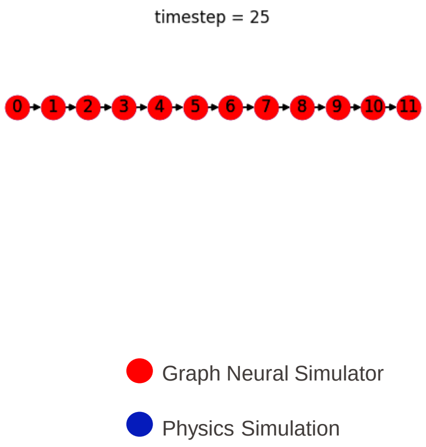
Assessing Model Performance in Generalization



Train : Train : 4, 5, 6, 7, 9, 10 masses
Test : 12 masses **(Extrapolation)**

GNN based Dynamics Model:
Details of Data-Driven Interaction Learning

Assessing Model Performance in Generalization

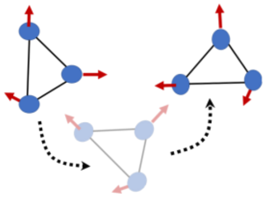


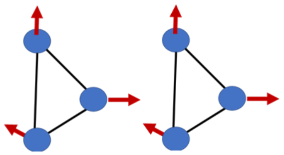
Research Gap
Purely Data Driven GNNs
1) Prone to Error-Accumulation For Long Rollouts
2) Unsatisfactory Generalization

Proposed Method: PI-GNN

1) Novel Architecture with Symmetry Preservation, Momentum & Angular Momentum Conservation
2) Reinterpretation of Message Passing as Euler integration of Forward Newton Dynamics

Symmetry in Dynamical Systems:

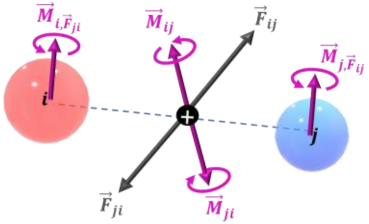




Rotation Equivariance : **Translation Invariance:**

Dynamical Vectors (Forces, Moments, Velocities etc. are Rotational Equivariant & Translational Invariant)

Conservation Laws in Dynamical Systems:



Conservation of Linear & Angular Momentum:
For 2 interacting Bodies with internal forces
- Linear momentum is conserved
- Total angular momentum is conserved

- **Conservation of linear momentum implies equal and opposite interaction forces between two bodies.**
- **Conservation of angular momentum implies equal and opposite total torques on each body.**

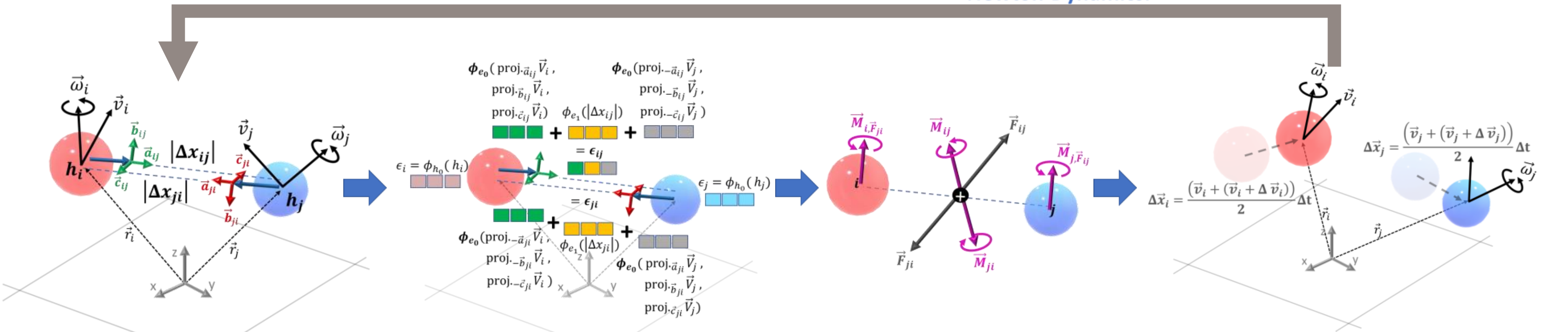
These biases are general and therefore are applicable to broad range of systems, PINNs on the other hand require system specific PDE knowledge

Proposed Method: PI-GNN

1) Novel Architecture with Symmetry Preservation, Momentum & Angular Momentum Conservation
2) Reinterpretation of Message Passing as Euler integration of Forward Newton Dynamics

Single Message Passing Layer of PI-GNN:

Message Passing:
Single Step Forward
Newton Dynamics.



3D Local Reference Frame Defined for Each Edge

Symmetry Bias

Encode Vectors & Scalar Features Separately.

- Project Vectors on Local Reference Frame to get New Scalars.

Symmetry Bias

Decode Internal Dyn. Vectors:
(Internal Forces & Moments)

- Decode such that conservation of Linear & Ang. Momentum is guaranteed

Conservation Bias

Update Node State:

- Single Step Forward Newton Dynamics

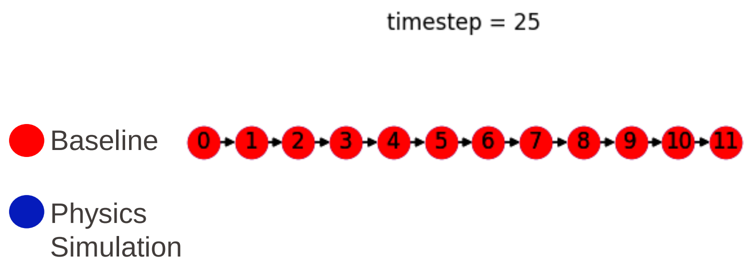
Forward Dynamics Bias

Generalization : Larger Systems

GNS v/s PI-GNN (proposed)

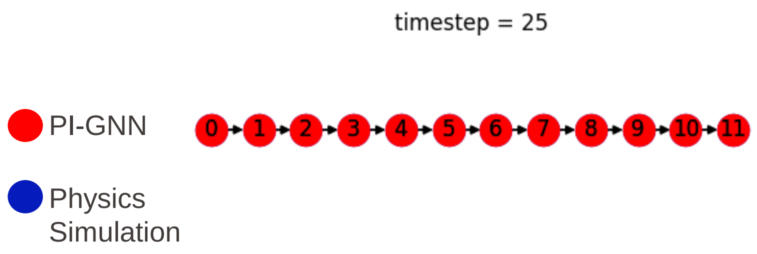
Train : 1000 time-step trajectories of 4, 5, 6, 7, 9, 10 masses

Baseline



12 masses
(+2)

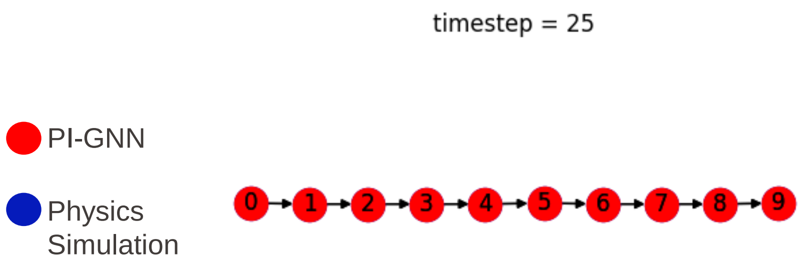
PI-GNN



12 masses
(+2)

Generalization : New Boundary conditions

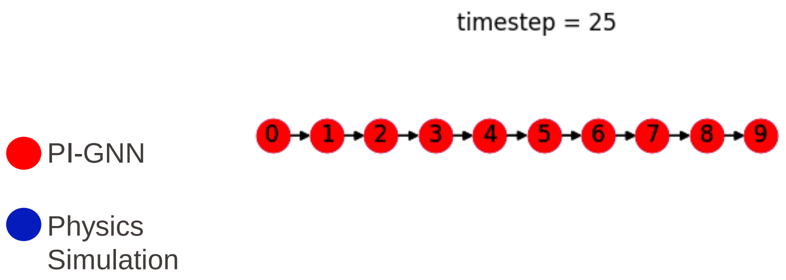
Train : 1000 time-step trajectories of 4, 5, 6, 7, 9, 10 masses



10 masses
&
3 nodes fixed

Generalization : New Boundary conditions

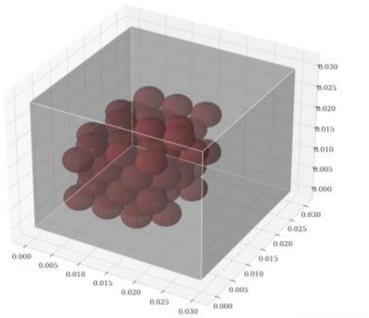
Train : 1000 time-step trajectories of 4, 5, 6, 7, 9, 10 masses



8 masses

Transition to Chaotic Spring-Coupled Double Pendulum

Application to 6 DOF Collision Dynamics



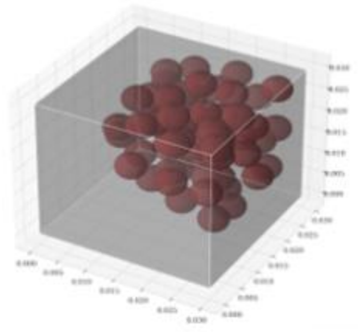
SIMULATED TRAJECTORIES WITH MFix DEM SOLVER

TRAINING DATA:

4 cases with **different initial velocity** of **spheres with 6 DOF colliding** with

- with **rough walls of a box** (coeff. of friction : 0.1), coeff of restitution : 0.9
- with **other spheres** (coeff. of friction : 0.1), coeff of restitution : 0.9

Application to 6 DOF Collision Dynamics



TRAINING DATA:

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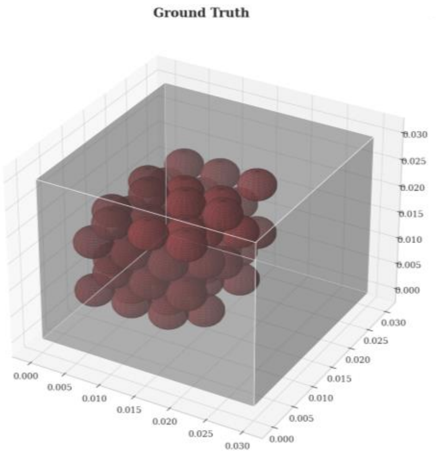
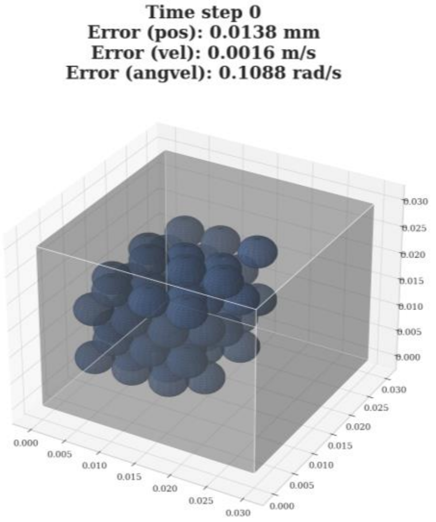
- with **rough walls of a box** (coeff. of friction : 0.1), coeff of restitution : 0.9
- with **other spheres** (coeff. of friction : 0.1), coeff of restitution : 0.9

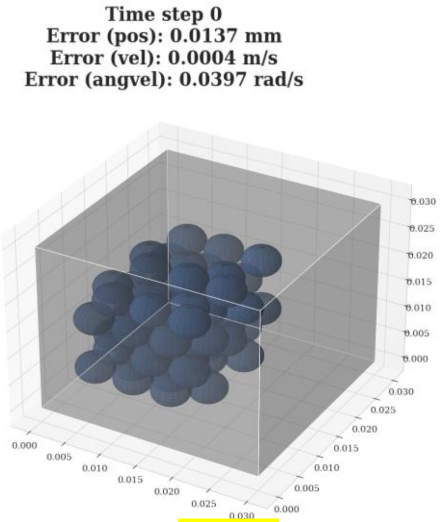
GENERALIZATION : 3x Initial Velocity



GROUND TRUTH
(DEM SIM.)



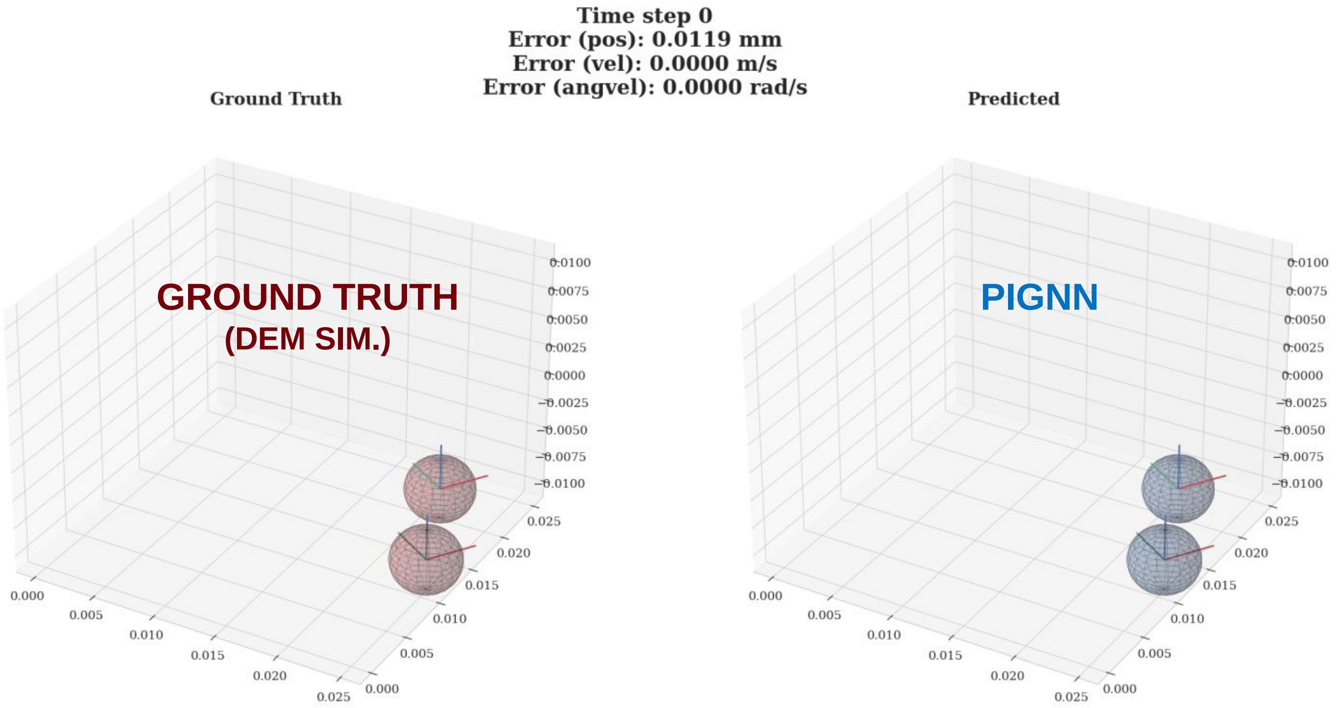
GNS
(Baseline)



PIGNN
(Ours)

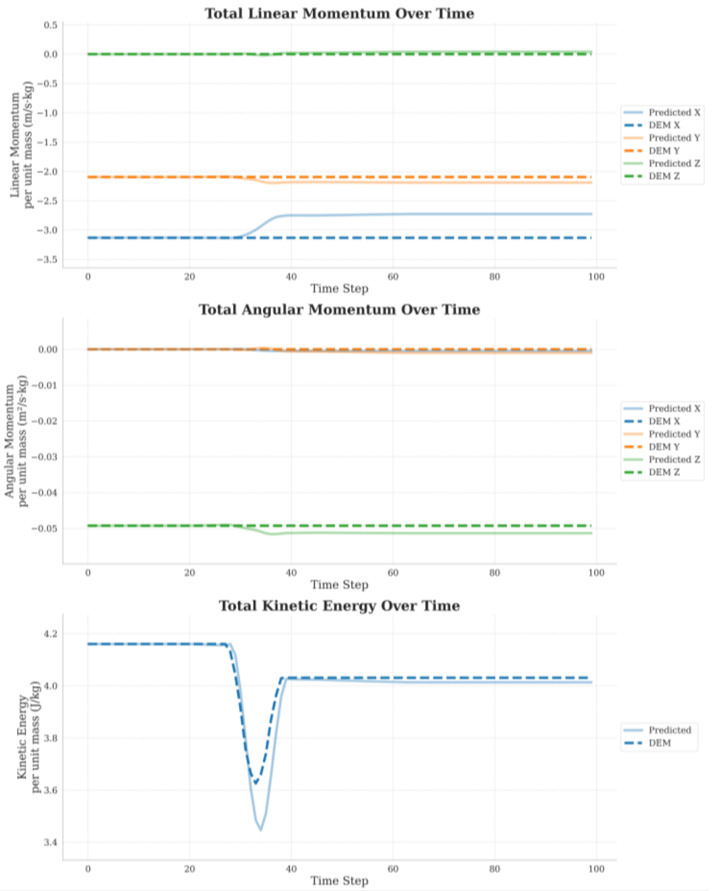
Linear & Angular Momentum Conservation

Experiment : A closed system of two particles undergoing inelastic collision
(training data: 4 cases of box collisions same as before)

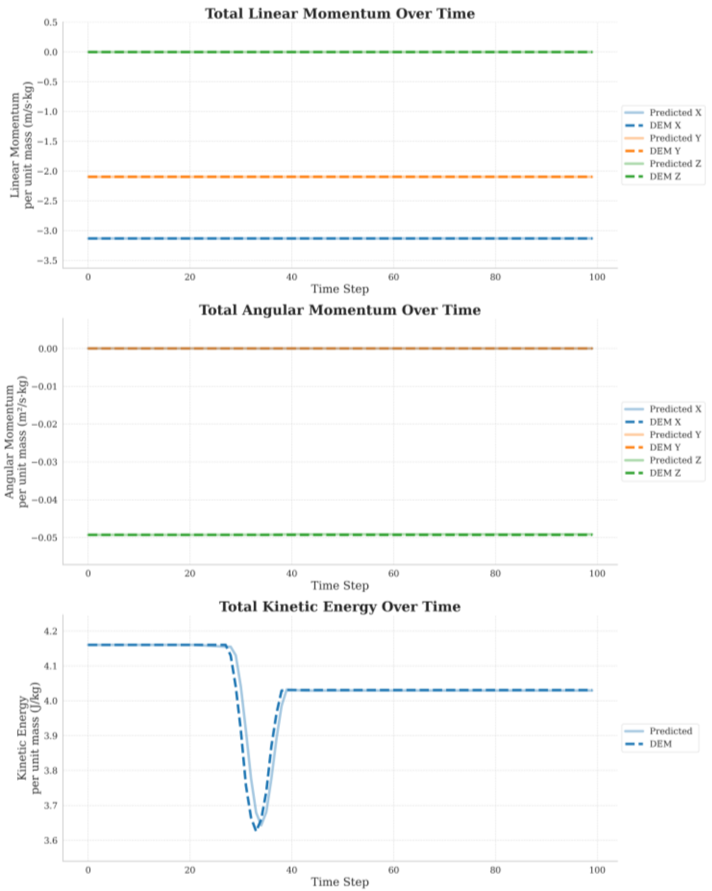


Linear & Angular Momentum Conservation

GNS (16 layer, 5 time step history)

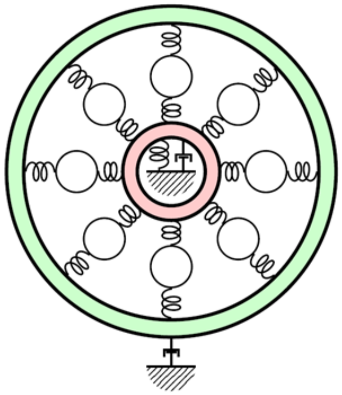


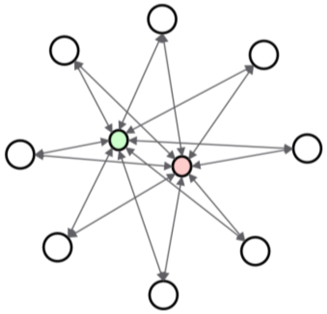
PIGNN (1 layer, 1 time step history)



Application to Industrial Multi-Body Systems

2D dynamic model of Rolling Element Bearing





Graph

PI GNN

Trajectory data

- 2D dynamic lumped bearing model, (based on P. K. Gupta, 1979)
- Differential equations of motion
- Lundberg & Palmgren model for Hertzian contact
- N209 CRB bearing (line contacts)

Application to Industrial Multi-Body Systems

Data: 2D dynamic model of Rolling Element Bearing

TRAININIG DATA :

BEARINGS : 13, 14 and 16 Rolling Elements Configurations

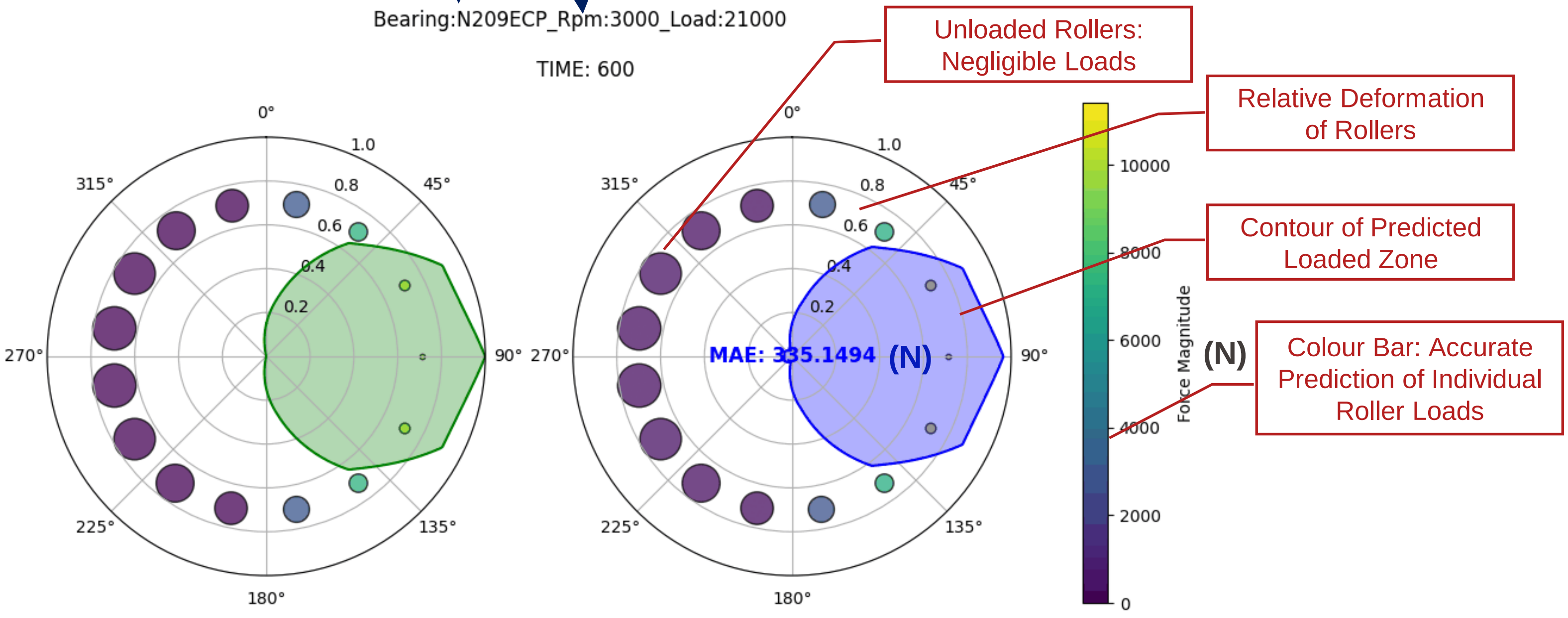
RPM : 300, 333, 428, 500, 600, 1000, 1499

LOADS: 5000, 7000, 9000, 11000, 13000, 15000, 17000

Untrained Bearing Configuration

RPM: **Outside** Training Data

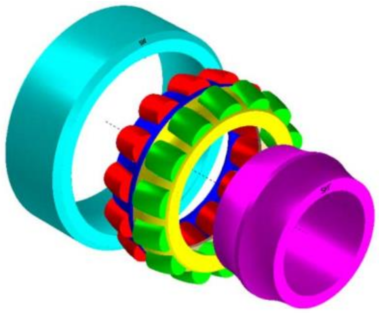
Load: **Outside** Training Data



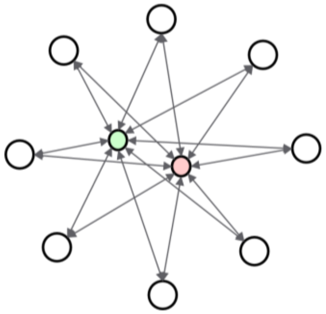
Ground Truth **Prediction**

Application to Industrial Multi-Body Systems

Data: Mesh based FEA + CFD Simulation of Lubricated Bearing



FEA SIMULATION



Graph

PI GNN

Trajectory data

- Damping due to lubricant
- Contact stresses on the rollers
- 3-D structural forces on the rollers and raceways.

Application to Industrial Multi-Body Systems

Data: Mesh based FEA + CFD Simulation of Lubricated Bearing

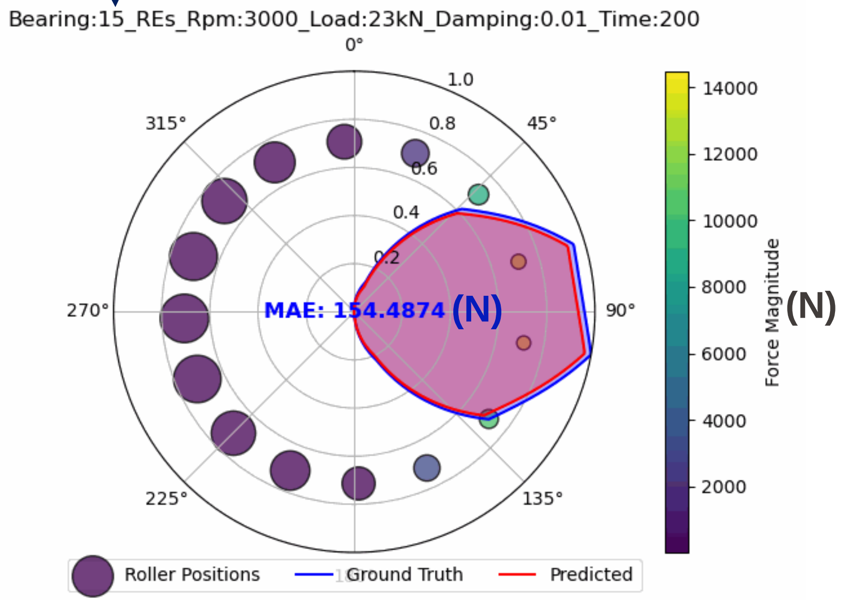
TRAININIG DATA :

BEARINGS : 13, 14 and 16 Rolling Elements Configurations
RPM : 300, 333, 428, 500, 600, 1000, 1499
LOADS: 5000, 7000, 9000, 11000, 13000, 15000, 17000

Untrained Bearing Configuration

RPM: **Outside** Training Data

Load: **Outside** Training Data



Meshless

Fast Inference

Long stable Rollout

Conclusions:

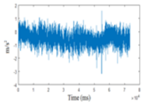
OUTPUT

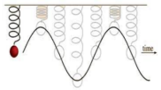

On-line Dynamics Prediction as a function of Changing Operating Conditions.


Interpretable & Explainable dynamics


Long trajectory roll-out & stable error accumulation

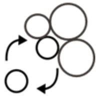
INPUT DATA

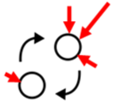

Noisy input data



Learning from trajectory without parameters as input

GENERALIZATION

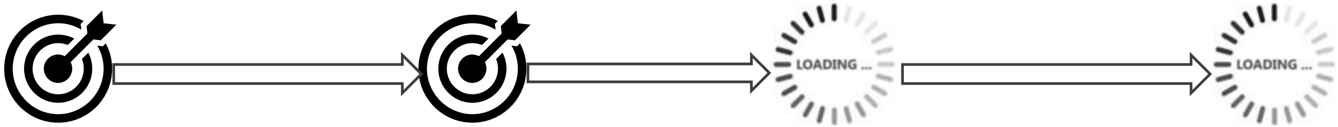

Extrapolation to Unseen Configurations


Generalization to unseen operating conditions

PIGNN

- **Applicable to broad range of dynamical systems**
- **Conservation of Momentum & Symmetry Preservation**
- **Long Stable Dynamics Rollouts**

Next Steps :



Online Surrogate Model trained on Lumped Parameter Models

Online Surrogate Model trained on FEA data

Online Dynamics from Measured Data

RUL prediction Based on Predicted Loads

THANK YOU