1st AI for Drinking Water Chlorination Challenge @ IJCAI-2025

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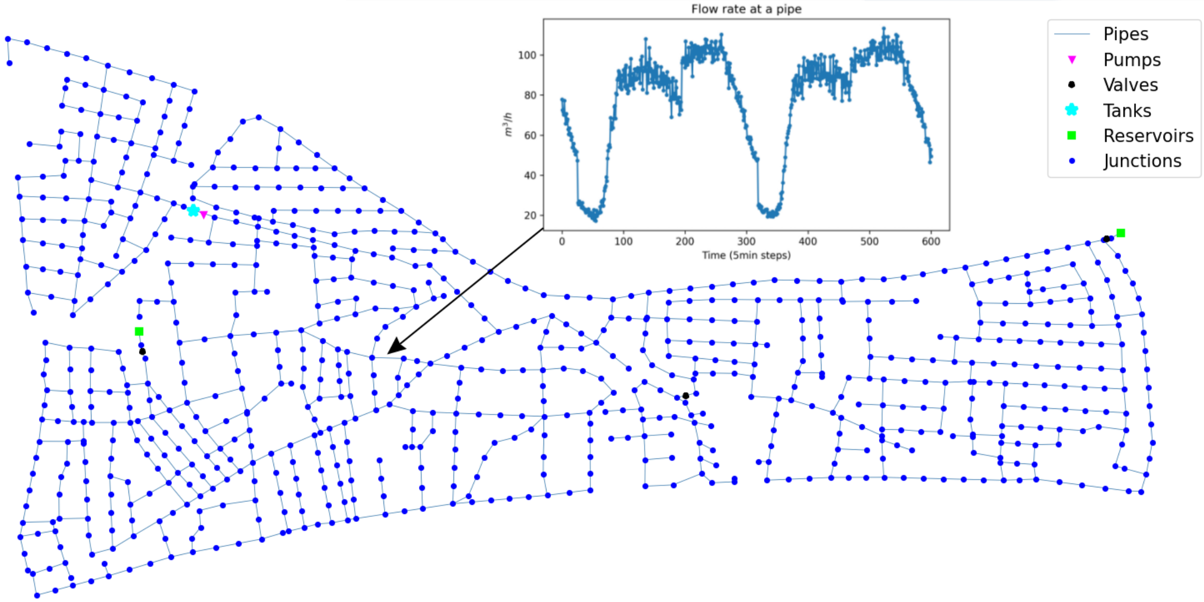
Water-Futures has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant agreement No. 951424)

Water Distribution Networks (WDNs)

- Providing access to drinking water
  - Crucial for society => Critical Infrastructure

- Modeled as **graphs**
  - Complex **spatio-temporal signals**
  - Demands, Pressures, flows, chemical concentrations, etc.

  => Described by **differential algebraic and partial differential equations**



$$\frac{\partial f}{\partial q} = R\,(X2 + R\,(2\;X3 + 3\;R\;X4))\;/\;|q|$$

$$\frac{\partial C_i}{\partial t} = -u_i \frac{\partial C_i}{\partial x} + r(C_i)$$

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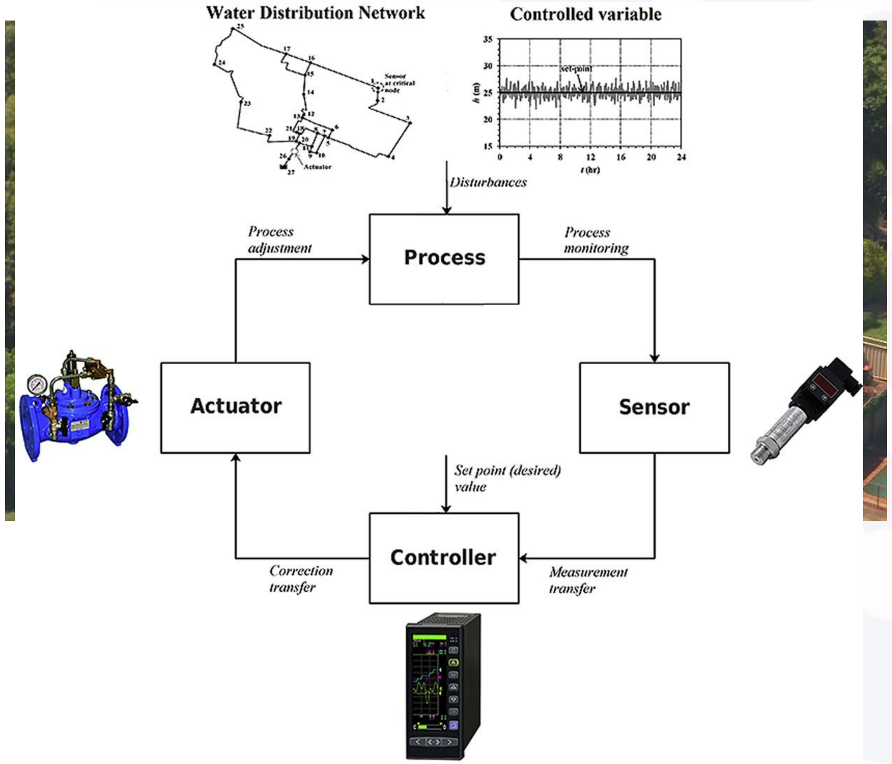
Tasks of Water Utilities

- Satisfy water demands at all times
- Ensure water quality – safe to drink
- Network planning
- Demand forecasting
- Leakage detection & localization
- Contamination detection & localization
- Control



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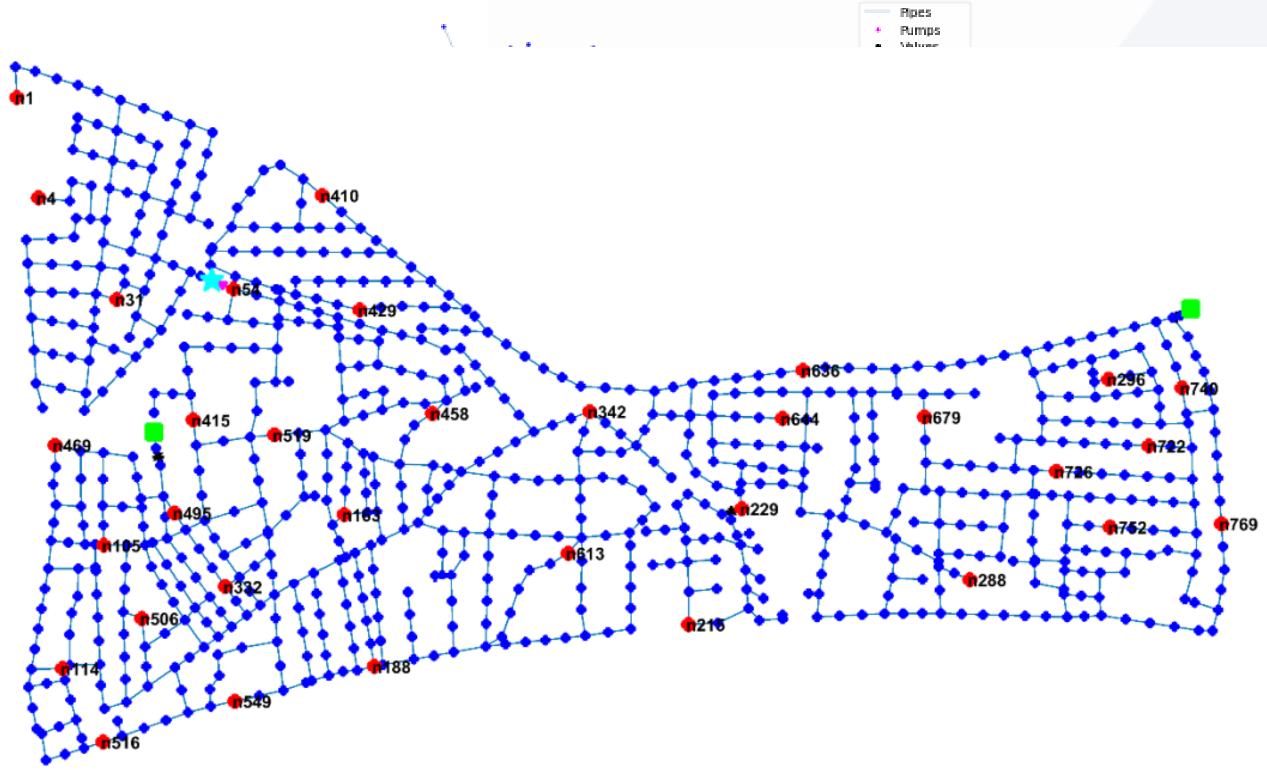
Challenges

- Lots of uncertainties
  - o Topology
  - o Measurements
- Sparse sensor readings
- Long time horizons
  - o Planning/Forecasting
  - o Policies
  - o Transport delay
- High-stakes application



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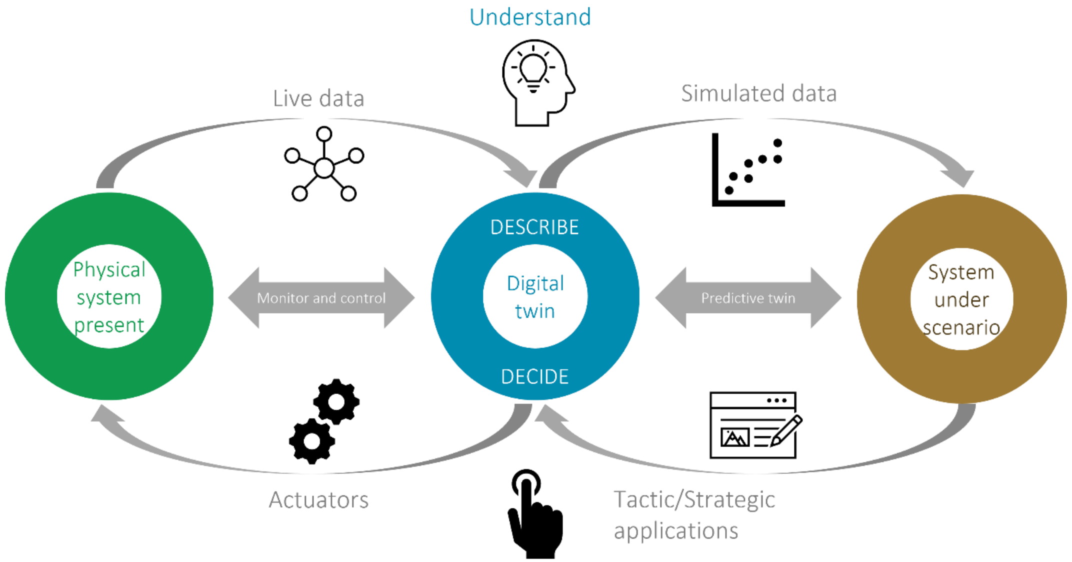
Applications of AI in WDNs

- *Operation of WDNs is non-trivial!*
  - e.g. different events, complex dynamics, etc.

  => How can AI help?

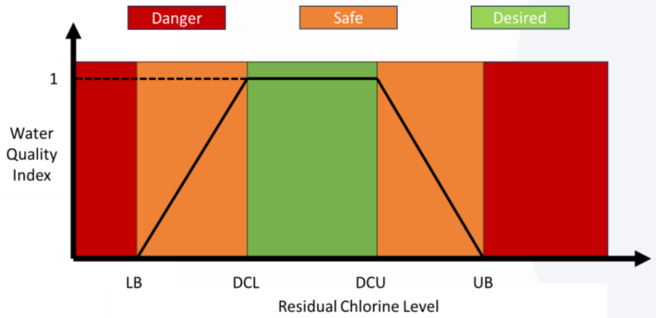
- Event detection and isolation
- Forecasting
- Control
- Surrogates & Emulators for complex simulations

  => e.g. Digital twins



Water Chlorination Control

- Chlorine is a typical disinfectant
  - Mitigate contaminations
  - Too much chlorine is poisonous!
  - Disinfection By-Products
- Injection of Chlorine into the network
  - Maintain safe chlorine levels
  - Respond to contaminations & hydraulic changes
- <u>Challenges:</u>
  - Uncertainties
    - Unknown substances & reaction (parameters)
  - Complex dynamics
- <u>*How can AI help?*</u>



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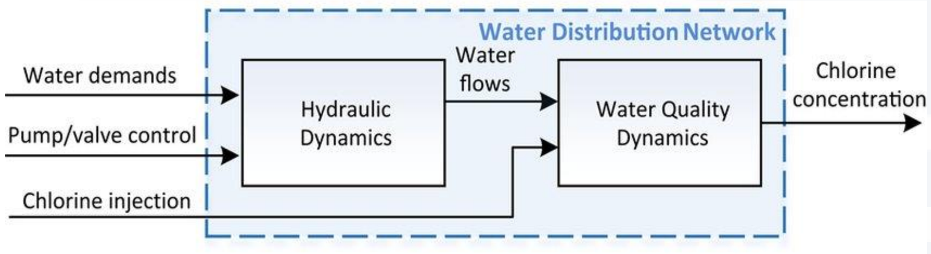
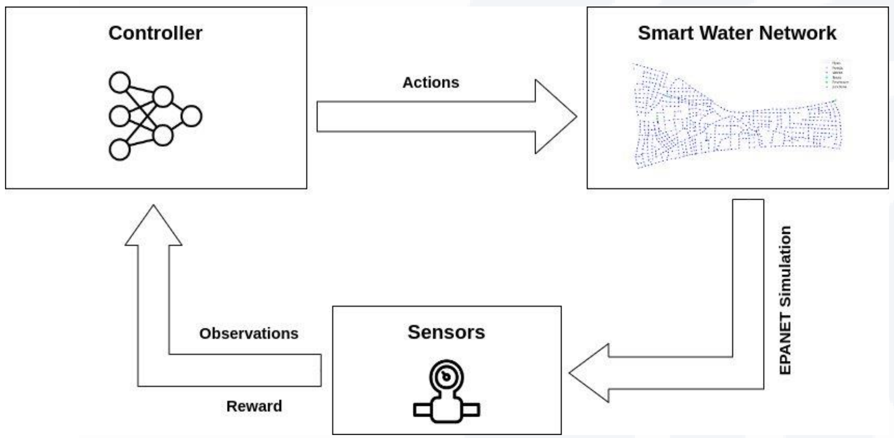
Potential of AI in Water Quality Control

- Surrogate models for complex dynamics
- State estimation under uncertainty
- Planning & Reinforcement learning for control
  - o Hydraulic actuators
  - o Chlorine booster stations
- ....





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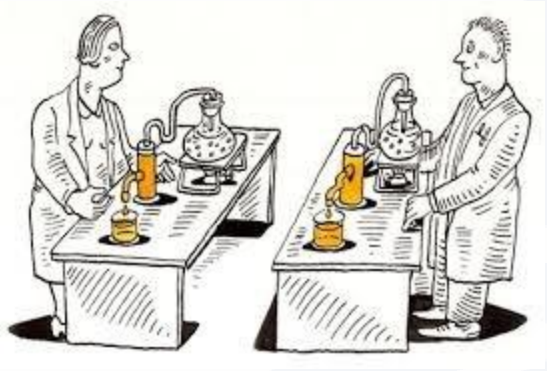
Lack of Benchmarks

- No benchmarks for chlorine injection control
- Benchmarks are essential for reproducible research and progress
    - Important for involving the AI community

=> Benchmark & Competition on *"AI for Water Chlorination Control"*



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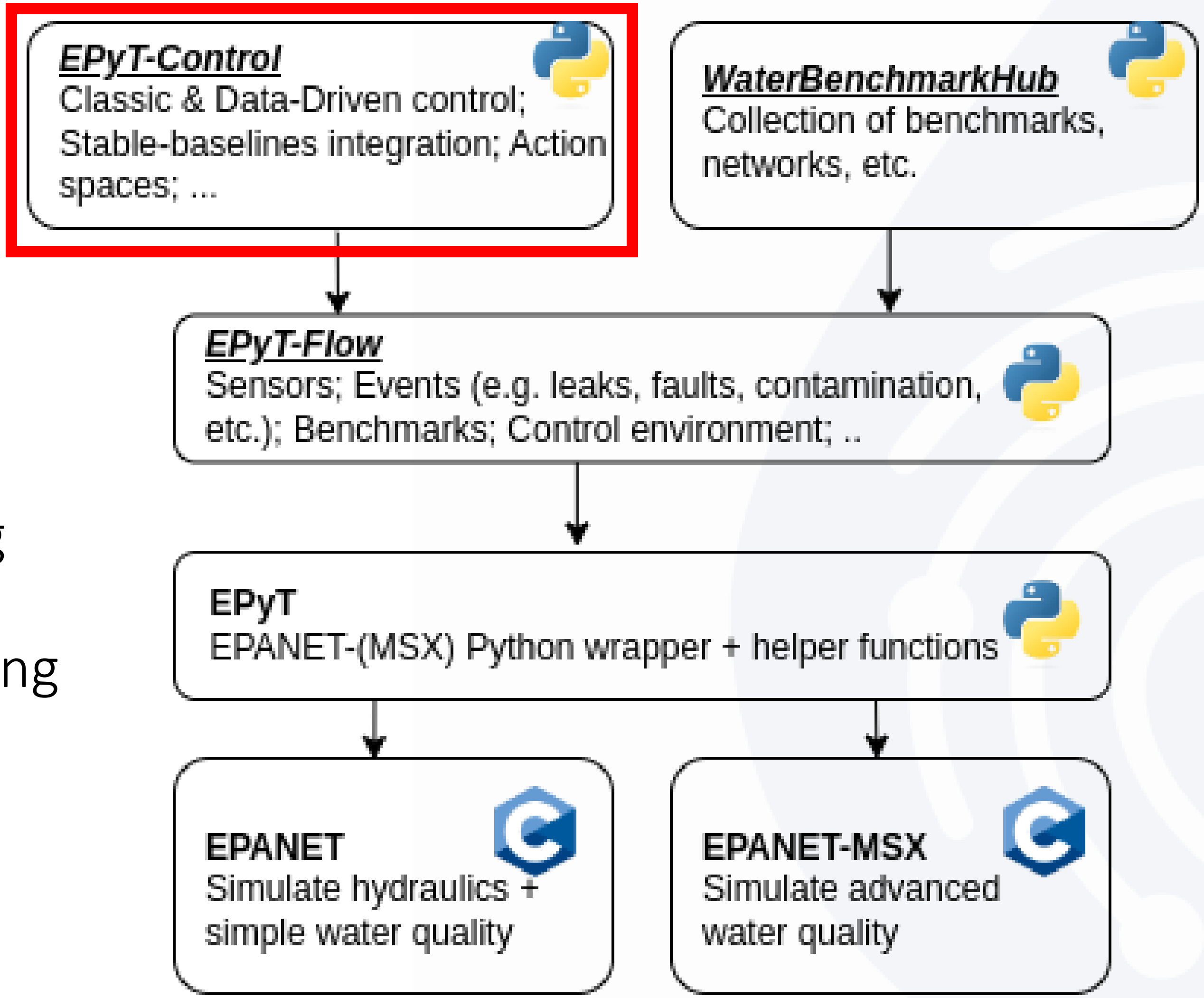
Software Backend

- EPANET & *EPANET-MSX*
  - Matlab + Python
- New toolbox **EPyT-Control**
  - Part of the EPyT family
  - Focus on control
    - PID control
    - ….
  - Interface for reinforcement learning
    - Integrates popular ML frameworks
  - State estimation and signal processing
    - Kalman filters
    - Event diagnosis
    - …



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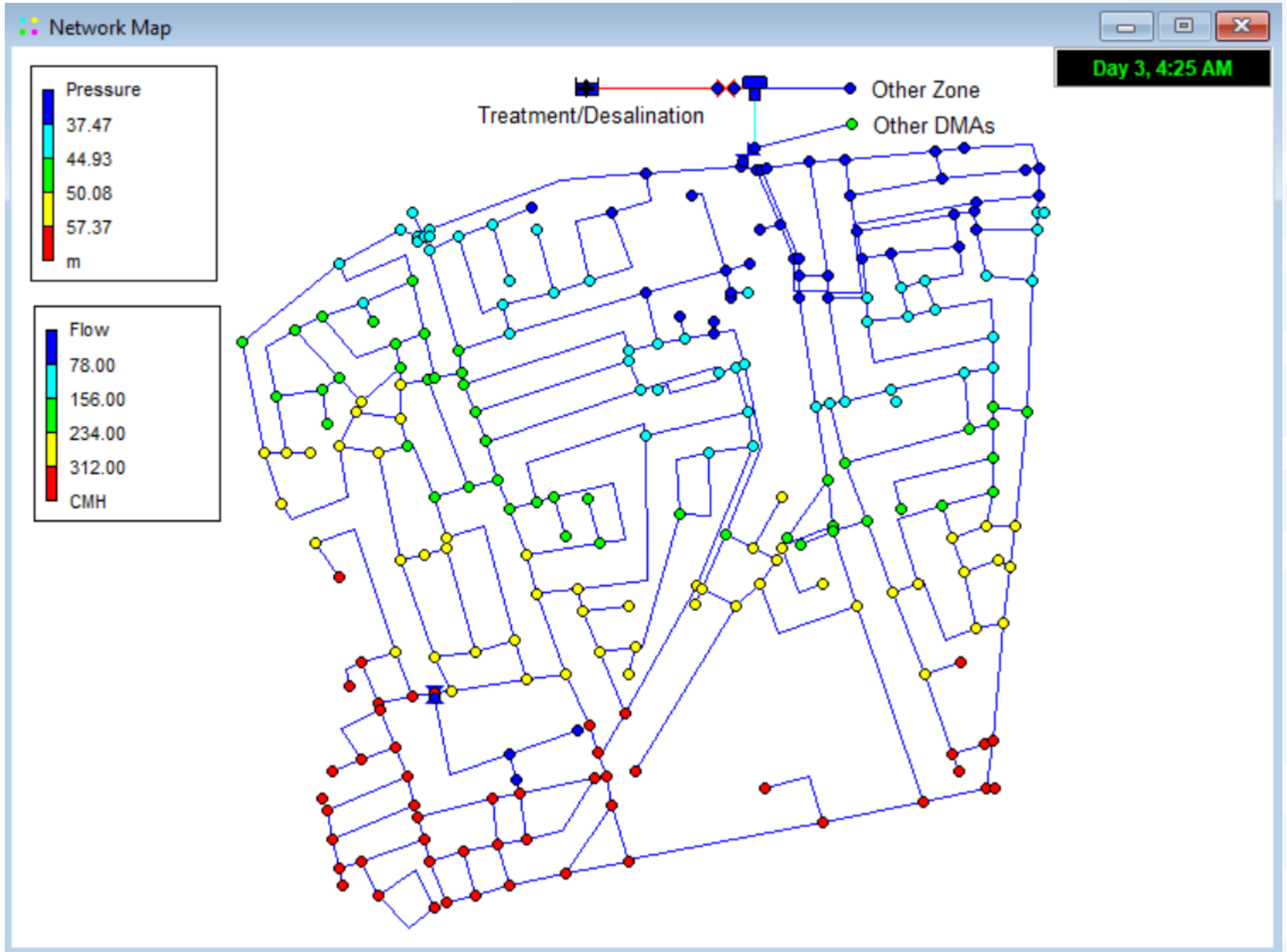
https://github.com/WaterFutures/EPyT-Control

Scenarios - Hydraulics

- **CY-DBP** realistic network
- Topology – 256 demand nodes, 335 pipes, 1 reservoir (WTP),
  1 elevated tank (T_Zone)
- Full-year simulation
- Hydraulic Time-Step of 5 min;
- Demand Dynamics
  - Diurnal pattern
  - Seasonal multipliers
  - Each node has a unique, STREAM-generated demand



P. Pavlou, et al., “A Comprehensive Virtual Testbed for Modeling Disinfection Byproduct Formation in Water Distribution Networks,” Engineering Proceedings 2024, Vol. 69, Page 33, vol. 69, no. 1, p. 33, Sep. 2024.

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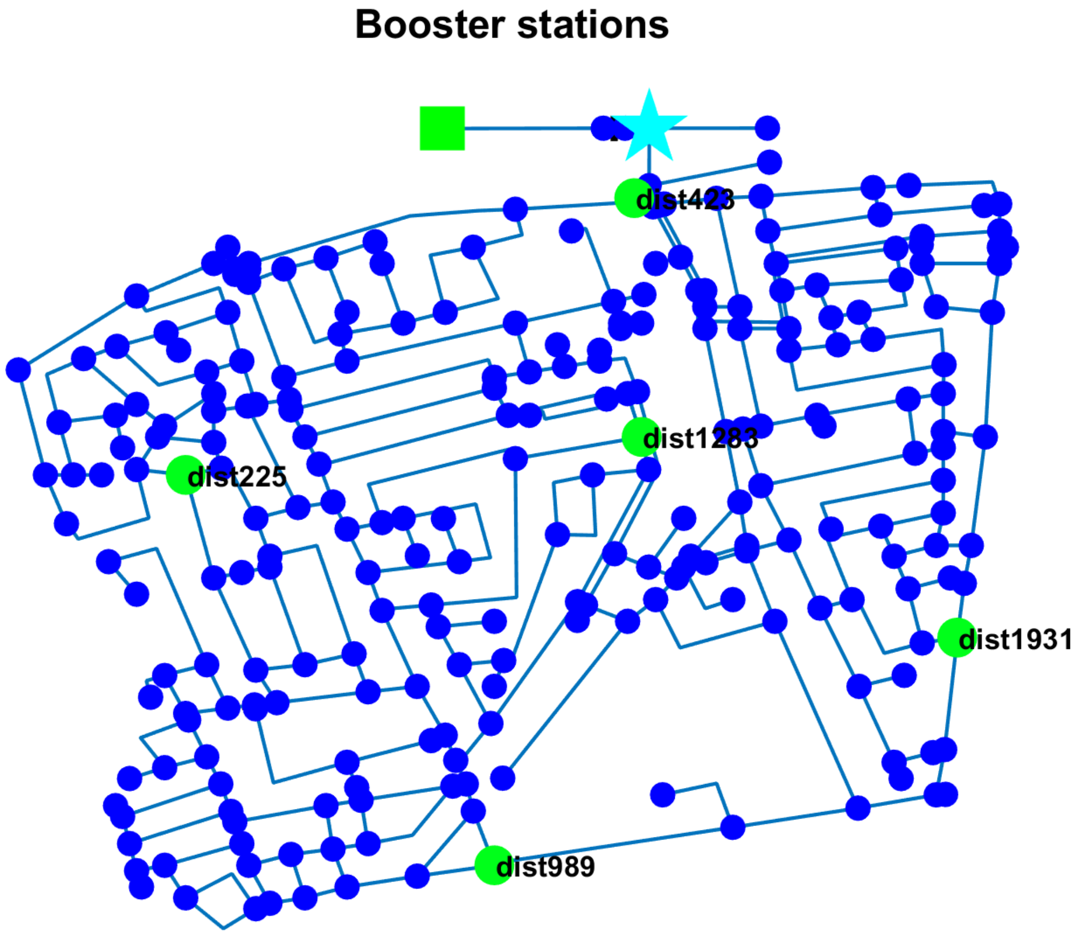
Scenarios - Quality

- Variable inlet chlorine
- Variable inlet organic matter (monthly) → variable chlorine decay
- Booster Control: 5 stations (Cl mass injection)
- **Hidden Challenges**: Random (waste water) contamination events
- Infection-Risk Evaluation Metric (based on QMRA)



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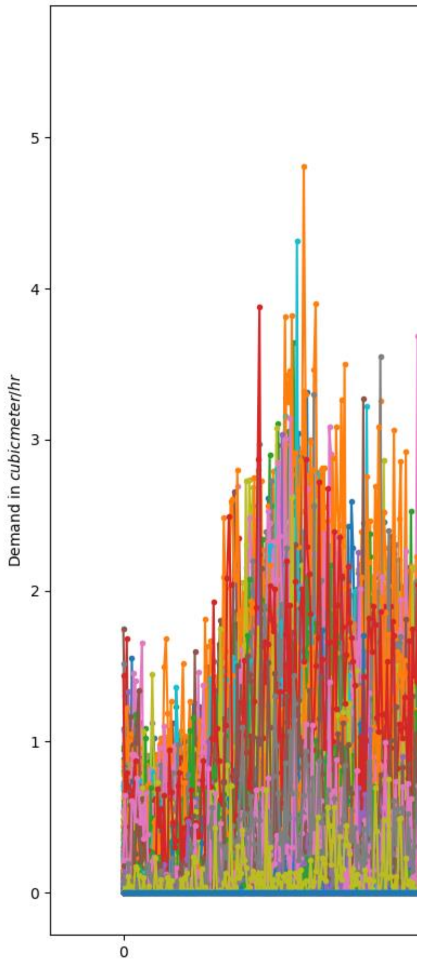
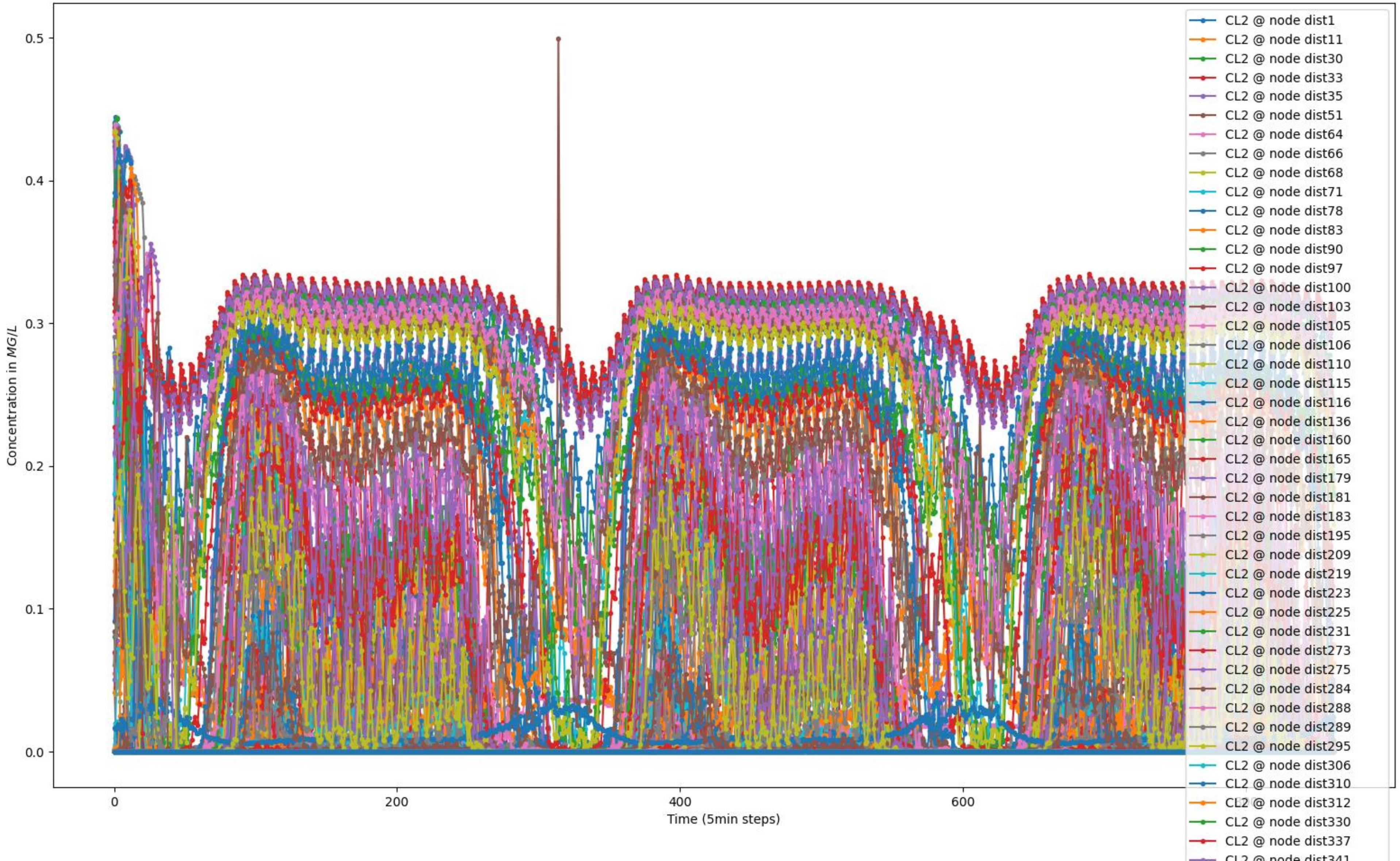
S. Paraskevopoulos *et al.*, "Modeling the health impact of wastewater contamination events in drinking water networks," *Journal of Cleaner Production*, vol. 479, no. January, p. 143997, 2024.

Dynamics for 3 Days

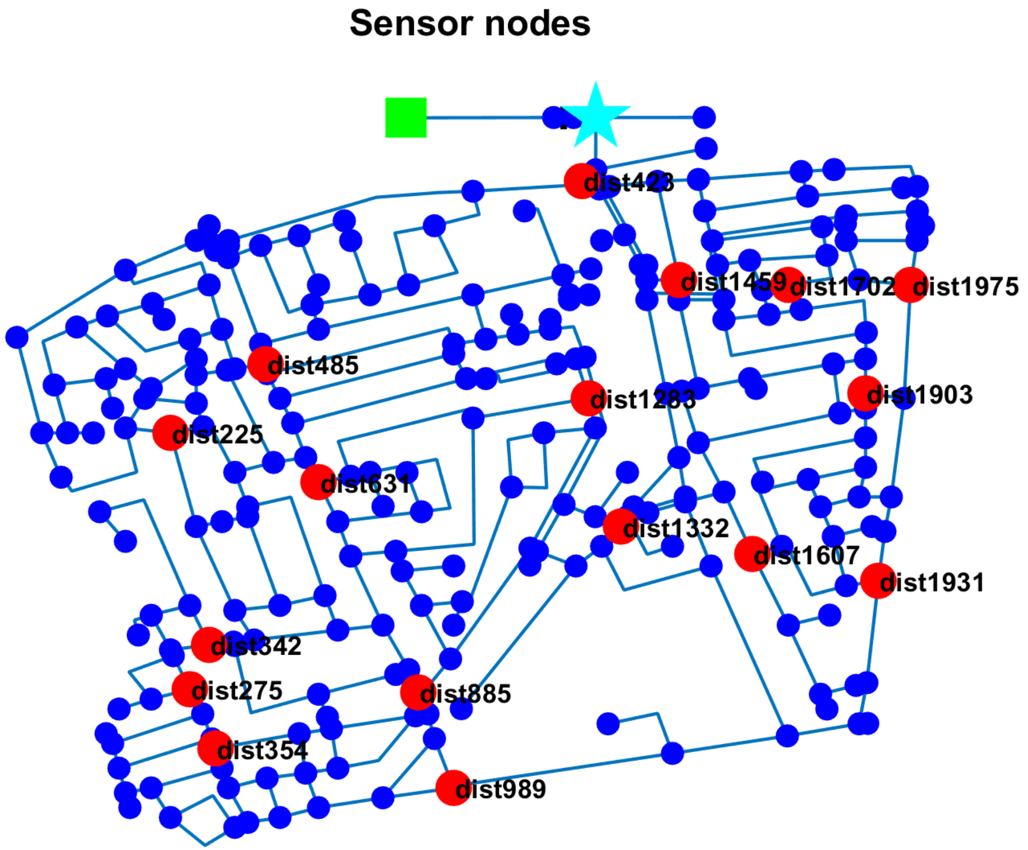




Scenarios – Control Inputs

- 17 Cl sensors + 2 flow sensors
- Optional:
  - Time
  - Network topology
  - ....

=> *How to control Cl booster stations?*



- 10 six days long scenarios with 1 contamination event
- One 365 days long scenario with 15 contamination events

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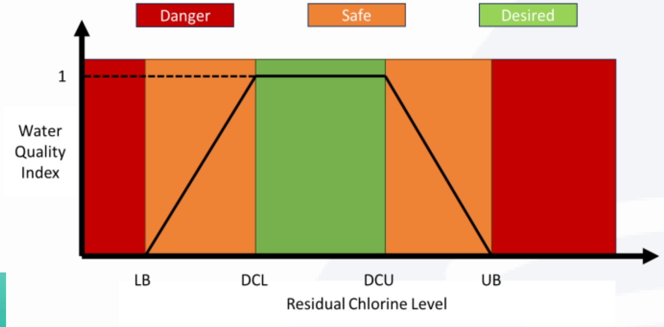
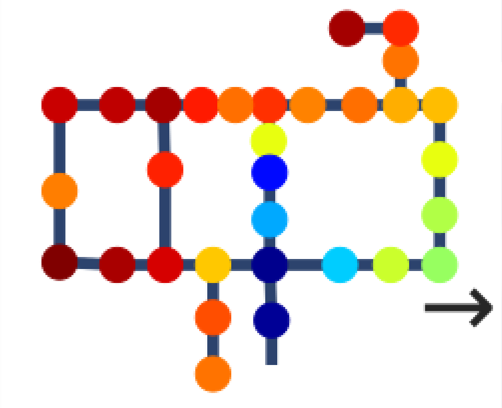
Evaluation – Multiple Criteria

- Secrete test scenario (365 days – 15 contaminations)
- Avg. local satisfaction of chlorine concentration bounds -- [0.2, 0.4] mg/L
- Avg. infection risk
- Fairness: Spatial variations of metrics
  - o Worst-case difference
- Cost of control: Total amount of injected chlorine
- Injection pump operation constraints
  - o Max of avg. smoothness





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Results

- Six participating teams
- Different approaches:
  - o Deep Reinforcement Learning
  - o Rule-based Methods
  - o Evolutionary Methods
  - o Control Theory
- Raking for multi-objective problem

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Results -- Ranking

Team ID	Cost of control	Control smoothness	Cl bound violations	Cl bound violations fairness	Infection risk (avg. over all contamination events)
1	31048978.0	5.937	0.103	0.177	6.656
5	209191.72	0	0.171	0.199	9.082
3	19098485.02	50.36	0.150	0.331	8.067
2	0	0	0.171	0.199	9.085
4	0	0	0.171	0.199	9.085
6	-	-	-	-	-

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Top 3 Submissions

- **Team 1:**
  - PPO, MPC, and Rule mining
  - *Best method:* Rule mining with simple surrogate model (LSTM for predicting future Cl concentrations)
- Team 5:
  - Evolutionary Surrogate-Assisted Prescription (ESP) for surrogate models (LSTM)
  - Neuroevolution of Augmenting Topologies (NEAT) for learning policies
- Team 3:
  - Data-Enabled Predictive Control (DeePC) + fallback PID control
  - Reconstructs system dynamics from historical input–output trajectories encoded via Hankel matrices

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Summary & Outlook

- AI for water quality control – control Cl booster stations
  - o Complex and difficult problem
  - o Surrogates super important!

- Scenario generator
- 2nd challenge next year
  - o More realistic scenarios (background leakages, sensor faults, etc.)
  - o Sensor + booster station placement
  - o More scenarios + scenario generator
    - Avoid overfitting of evaluation metrics!
  - o "Live" leader board
  - o More "complex"/"advanced" evaluation scores (not only averages)
  - o .....

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https://github.com/WaterFutures/AI-for-Drinking-Water-Chlorination-Challenge-IJCAI-25