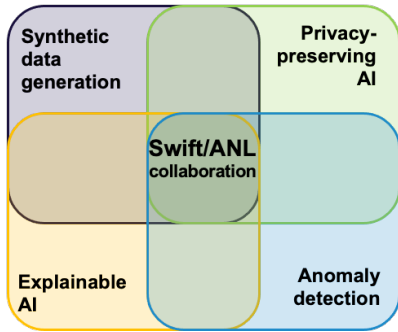


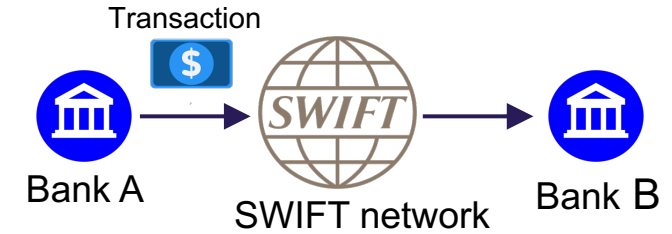
AI/ML for generative models and acceleration of scientific workloads

Generative AI for unstructured data



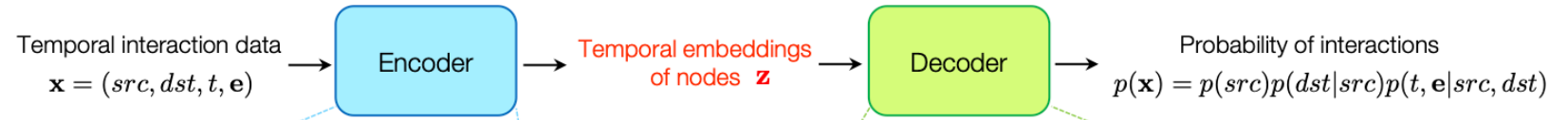
Bank-to-bank Transaction data

Date & Time	Currency	USD Eq.	Ordering BIC8	Beneficiary BIC8	Payment Route	Total Seconds Taken
Dec 31 2019 12:54:20	USD	42	TESTDEFF	AAAACATT	TESTDEFF;...;AAAAUS33;AAAACATT	300
Jan 1 2020 08:10:20	USD	13.37	DDDDIQBA	DDDDAEAD	DDDDAEAD;DDDDAEAD	666
Jan 1 2020 08:20:20	USD	1000.01	DDDDAEAD	DDDDUS33	DDDDAEAD;DDDDUS33	3600
Jan 1 2020 08:30:20	GBP	50.52245346	TESTDEFF	AAAAUS33	TESTDEFF;AAAAUS33;AAAACATT	10
Jan 1 2020 08:35:20	EUR	14.69323405	ZZZZFRPP	BBBBGB2L	ZZZZFRPP;BBBBGB2L	30
Jan 1 2020 08:42:03	JPY	7.252143432	ZZZZFRPP	CCCCBEBB	ZZZZFRPP;ZZZZJPJT;CCCCBEBB	120
Dec 31 2020 09:40:22	USD	42	ZZZZFRPP	AAAAUS31	ZZZZFRPP;ZZZZUS3N;AAAAUS33	10
Dec 31 2020 09:40:20	USD	13.37	ZZZZFRPP	ZZZZUS3N	ZZZZUS3N	
Dec 31 2020 09:42:42	USD	1000.01	TESTCNBJ	CCCCBEBB	TESTCNBJ;CCCCDEFF;CCCCBEBB	5



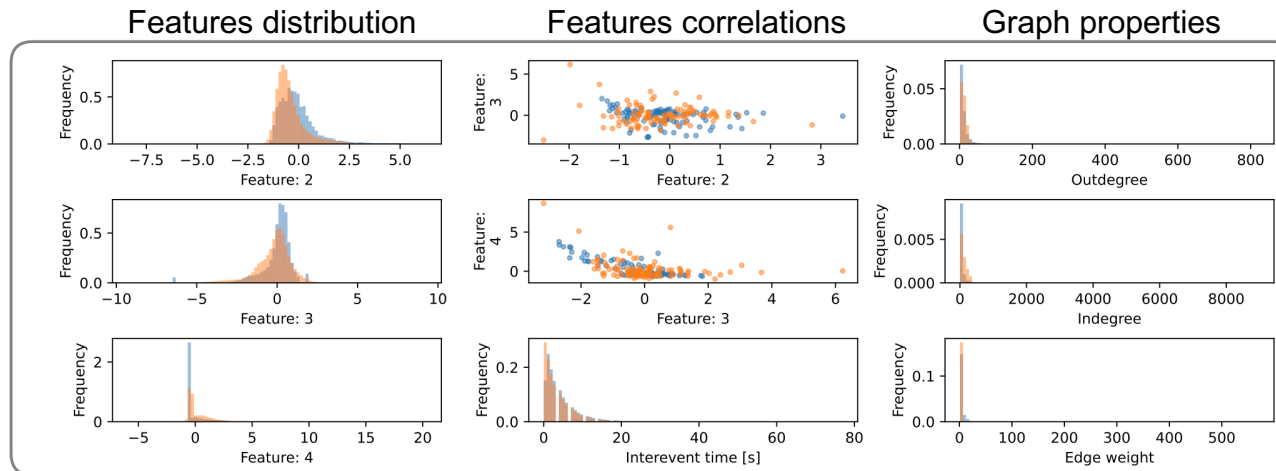
Graph data + Time series data + Tabular data = Temporal or Dynamic Graph data

Temporal Graph Generator:



Evaluation:

Real data vs Generated data



Temporal pattern

Neural Scaling of Graph Neural Networks (GNNs):

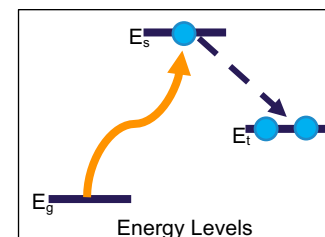
The performance of Transformer models keeps improving as they get bigger.

How well do GNNs scale?

ML to accelerate scientific workloads

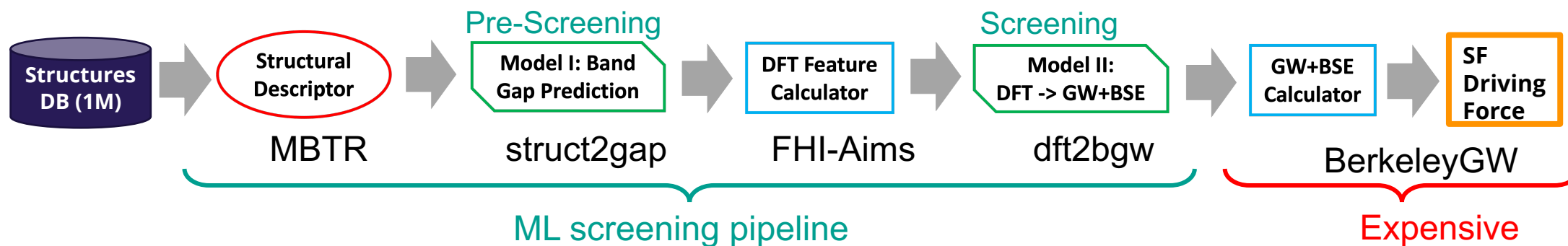
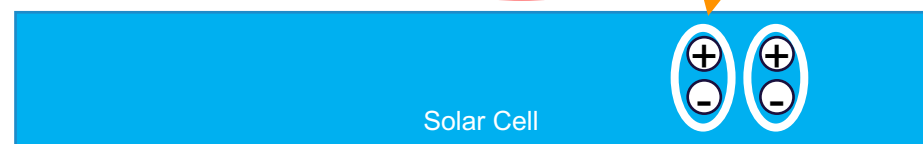
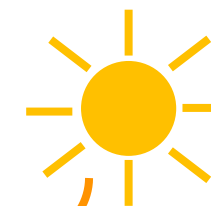
MatML ESP project:
discover new materials that exhibit intermolecular Singlet Fission (SF), in order to increase the efficiency of organic solar cells.

Large band gap $E_s - 2E_t$
+
High SF driving force
↓
Good SF candidates



Singlet Fission Driving Force:
 $E_s - 2E_t > 0$

Shockley-Queisser limit:
33.7% efficiency @ 1.34 eV



- Model 1: **struct2gap** – Gaussian process, GNN
- Model 2: **dft2bgw** – SISSO
- **Active learning**: used to determine which structures to add to the models' training sets
- **Workflow manager**: Balsam – orchestrate models' training and inference, launch all calculations, analyze results.