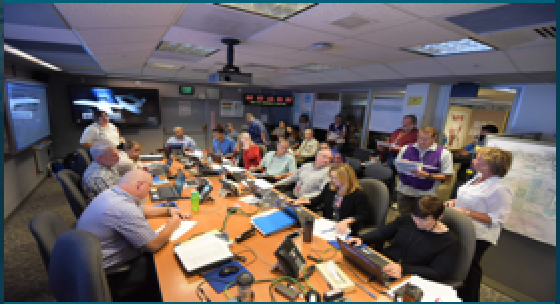
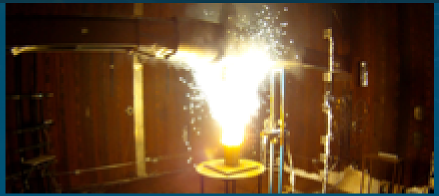
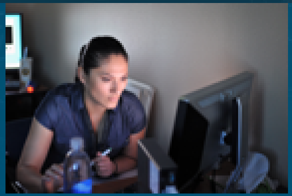
SAND2021-12019C

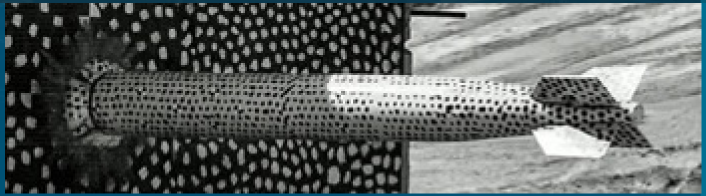
Sandia National Laboratories

Machine learning of Physics-Informed Graph Neural Networks from TCAD models









Presented By

Andy Huang for MMLDT-CSET 2021

on work w/ Nathaniel Trask (SNL), Suzey Gao (SNL), Shahed Reza (SNL), Ravi Patel (SNL), Christopher Brissette (RPI), and Xiaozhe Hu (Tufts)

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Overview

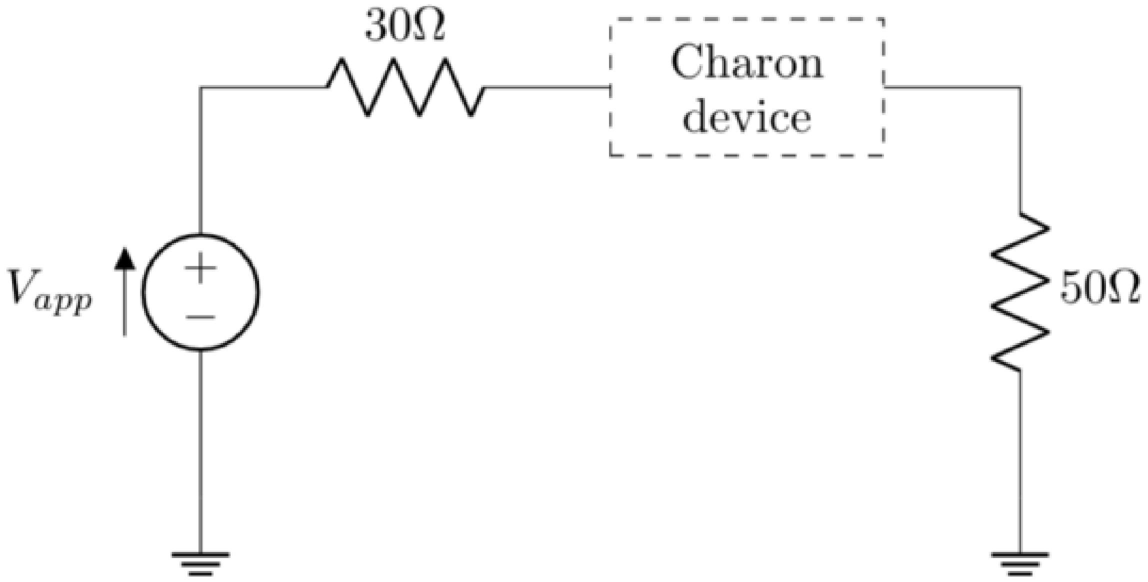
1) Multiphysics problems and reduced-order models

2) Desirable structures: physics conservation laws

3) Data-driven Discrete Exterior Calculus (DDEC) on a graph as a machine-learning framework with desirable structure

4) DDEC graph structure from TCAD simulation

Large picture: Multiphysics (expensive) electrical systems example




```
Resistor Circuit Netlist - lower level.
****************************************
R1          1 2 30
vconnectL   2 0 1.0
vconnectR   3 0 3.0
R2          3 0 50
VR          1 0 5.0
.DC R1 5 5 0
.options nonlin nox=1
.options device debuglevel=-100
.END
```

Xyce™ PARALLEL ELECTRONIC SIMULATOR

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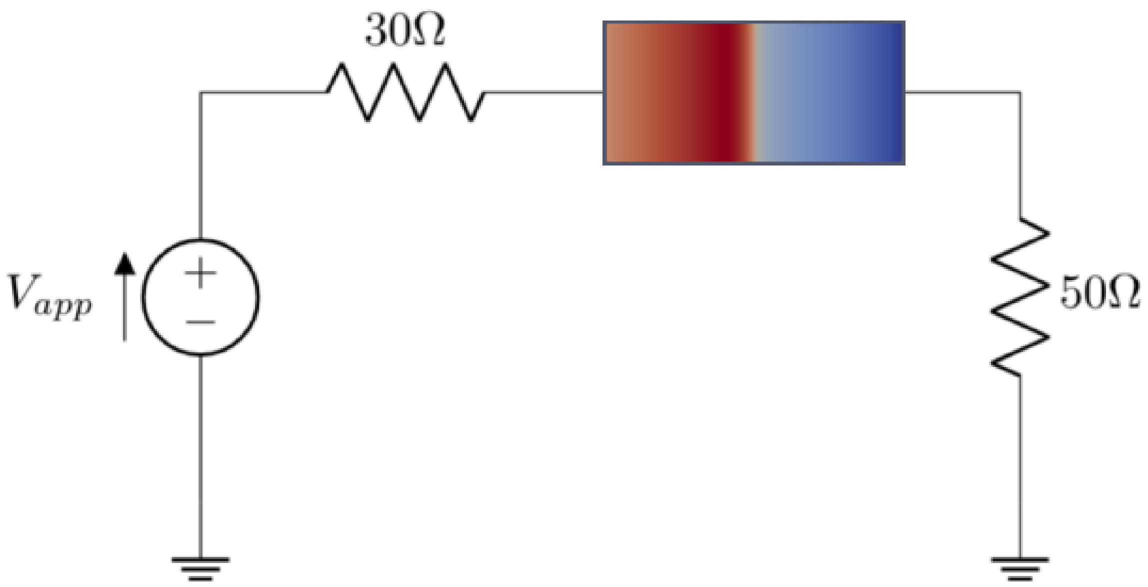
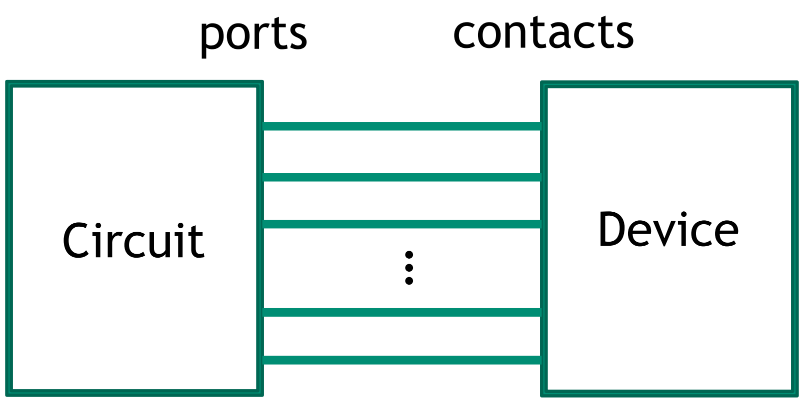
input decks

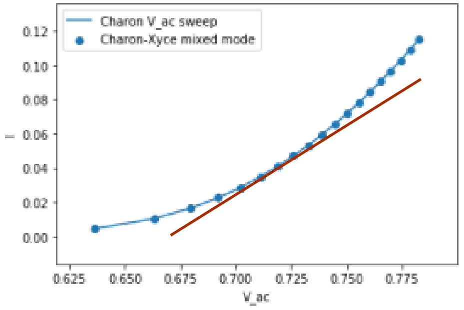
```
Import State File pndiode.dd.exo at index 1

tpetra is on

start output parameters
      Output State File resistorX_pndiodeC_resistorX.dd.exo
end output parameters

start Physics Block Semiconductor
      geometry block is silicon
      standard discretization type is drift diffusion gfem
      material model is siliconParameter
end Physics Block Semiconductor

start Material Block siliconParameter
      material name is Silicon
      relative permittivity = 11.9

      start Carrier Lifetime Block
            electron lifetime is constant = 1e-11
            hole lifetime is constant = 1e-11
      end Carrier Lifetime Block

      start step junction doping
            acceptor concentration = 1e16
            donor concentration = 1e16
            junction location = 0.5
            dopant order is PN
            direction is x
      end step junction doping
end Material Block Silicon Parameter

BC is mixed mode via current for anode on silicon as node named vconnectL in netlist r\
esistorX_pndiodeC_resistorX.cir with initial current -1e-3 with initial voltage 1.5
BC is mixed mode via current for cathode on silicon as node named vconnectR in netlist\
 resistorX_pndiodeC_resistorX.cir with initial current 1e-3 with initial voltage 1.0

initial conditions for ELECTRIC_POTENTIAL in silicon is Exodus File
Initial Conditions for ELECTRON_DENSITY in silicon is Exodus File
Initial Conditions for HOLE_DENSITY in silicon is Exodus File

start solver block
  start tpetra block
    problem type is householder constrained steady state
    verbosity level is high
    start nonlinear solver wrms block
      absolute tolerance = 1.0e-10
      relative tolerance = 1.0e-8
    end
  end
end solver block
```

Large picture: Mixed-mode simulation coupling model fidelities





Xyce™ PARALLEL ELECTRONIC SIMULATOR



Expensive non-linear conductance matrix calculation at each Newton step

$$\begin{bmatrix} \frac{\partial I_1}{\partial V_1} & \frac{\partial I_1}{\partial V_2} \\ \frac{\partial I_2}{\partial V_1} & \frac{\partial I_2}{\partial V_2} \end{bmatrix}$$

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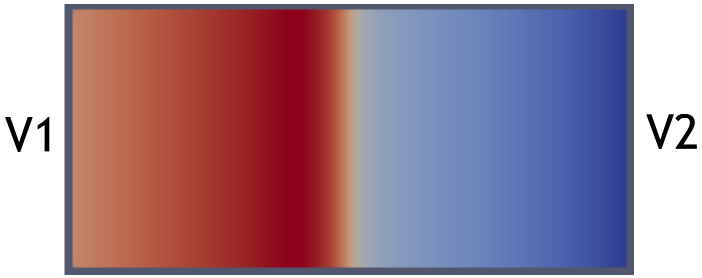
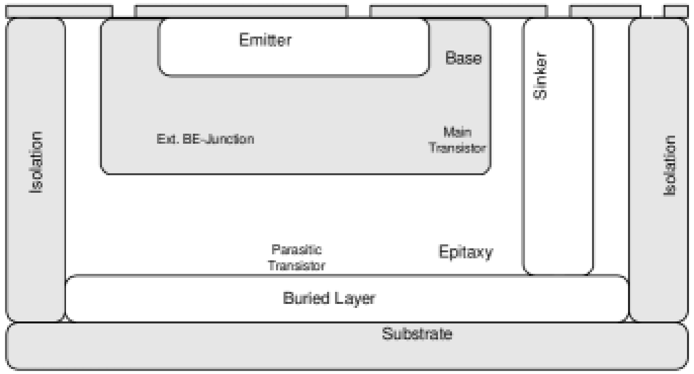


Large picture: Problem Statement

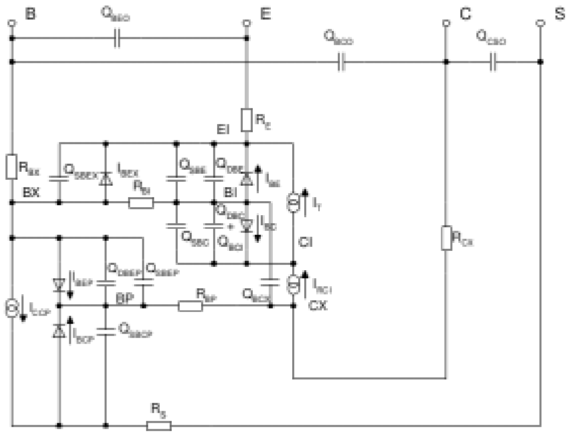
How do we transfer PDE-based physics knowledge to a reduced order model?

PDE-based physics model

$$\nabla \cdot \epsilon \nabla \phi = -(p - n + N_D^+ - N_A^-)$$
$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot (-\mu_n n E - D_n \nabla n) - R_n(n,p)$$
$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot (\mu_n p E - D_p \nabla p) - R_p(n,p)$$



Machine learned reduced order model



Traditional example from electrical engineering:

heuristically **identify local physical processes** and map input-output relationships to electronic components **assembled in a global circuit topology**.

Desired structure: Physics conservation laws

Many physical laws appear in **conservation form** as $\nabla \cdot \vec{J} = f$

- Kirchhoff's Current Law: $\sum_k I_{ik} = 0$
- Maxwell's equation: $\nabla \cdot \vec{E} = \frac{\rho}{\epsilon}$
- Incompressible flow $\nabla \cdot \vec{u} = 0$

Many physical laws and principles manifest through **potential theory**:

- Kirchhoff's Voltage Law: $\vec{V} = \nabla\phi$
- Darcy flow: $\vec{u} = -K\nabla\phi$ and $\nabla \cdot \vec{u} = 0$
- Gauge invariance: $\nabla\times\vec{A} = \vec{v}$ and $\vec{A} \to \vec{A} + \nabla f$

Related to **vector calculus identities**: $\nabla \cdot \left(\nabla\times\vec{A}\right) = 0$ and $\nabla\times(\nabla\phi) = 0$

Expressed in language of vector calculus (actually, operators on differential forms).

We choose to **express and embed these a priori in a network architecture.**

Data-driven Discrete Exterior Calculus

Topological structure with machine-learnable geometry (see Nathaniel Trask's talk @ **TIME**)

Topological chain complex:

$$C_0 \overset{\partial_0}{\leftarrow} C_1 \overset{\partial_1}{\leftarrow} C_2 \overset{\partial_2}{\leftarrow} \cdots \overset{\partial_{n-2}}{\longleftarrow} C_{n-1} \overset{\partial_{n-1}}{\longleftarrow} C_n$$

$$C^0 \overset{\delta_0}{\rightarrow} C^1 \overset{\delta_1}{\rightarrow} C^2 \overset{\delta_2}{\rightarrow} \cdots \overset{\delta_{n-2}}{\longrightarrow} C^{n-1} \overset{\delta_{n-1}}{\longrightarrow} C^n$$

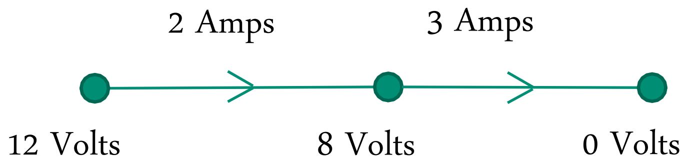
Geometric parameterization of differential operators:

$$d_k \coloneqq B_{k+1}\delta_k B_k^{-1}$$
$$d_k^* \coloneqq D_k^{-1}\delta_k^* D_{k+1}$$

Ohm's law: $\delta_0 V = RI$

Example:

Combinatorial (topological): $\begin{bmatrix} -1 & 1 & \\ & -1 & 1 \end{bmatrix} \begin{bmatrix} 12\ V \\ 8\ V \\ 0\ V \end{bmatrix} = \begin{bmatrix} R_1 & \\ & R_2 \end{bmatrix} \begin{bmatrix} 2A \\ 3A \end{bmatrix}$



$$R_1 = 2\Omega, R_2 = \frac{8}{3}\Omega$$

$\Rightarrow$ DDEC operator: $d_0 = \frac{1}{R}\delta_0$

DDEC Ohm's Law: $d_0 V = I$

Data-driven Discrete Exterior Calculus

For these circuit compact models, we will look for a graph topology.

Current i = edge vector (oriented)

Voltage v = edge vector (oriented)

Potential ϕ = nodal scalar

A = incidence matrix (branches to nodes)

Kirchhoff Voltage Law: $v \in im(A^T)$

Kirchhoff Current Law: $i \in ker(A)$

Tellegen's theorem: $(v, i) = 0$

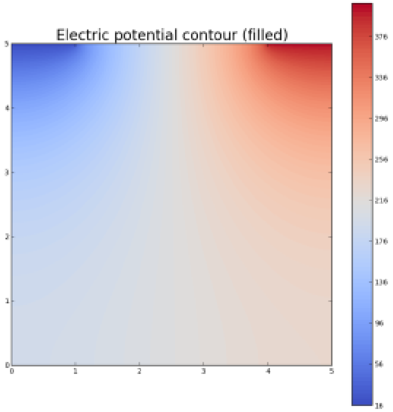
Objective: obtain graph from TCAD simulations and then dress it up for DDEC.

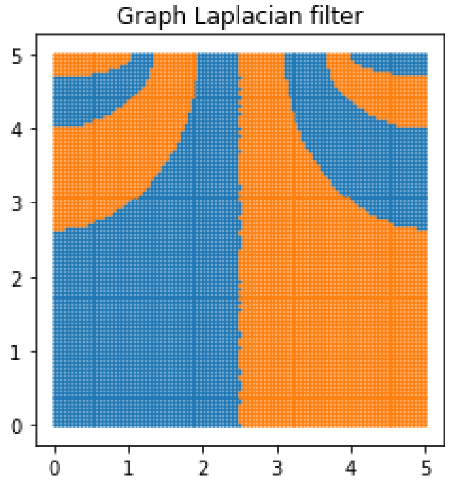
Large Picture Revisited: Workflow with DDEC

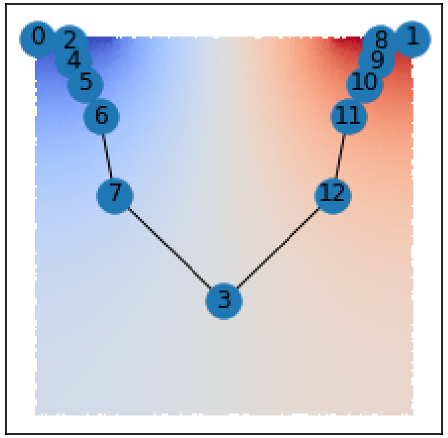
Prime Physics — Recognize Regions — Tailor Topology — Identify Interactions

Greedy Fiedler Spectral partitioning (obtain DDEC structure)

Physics-informed Graph Neural Network (trained DDEC model)








```
* Auto-generated netlist from NetworkX Graph
R0      0       1       1.0
R1      1       2       2.0
R2      1       2       2.0
R3      2       3       1.0
V1      3       0       2.0
.DC V1 0 2.0 0.2
.PRINT DC V(3) I(V1)
.END
```

CHARON

Mapper & scikit-tda

TensorFlow

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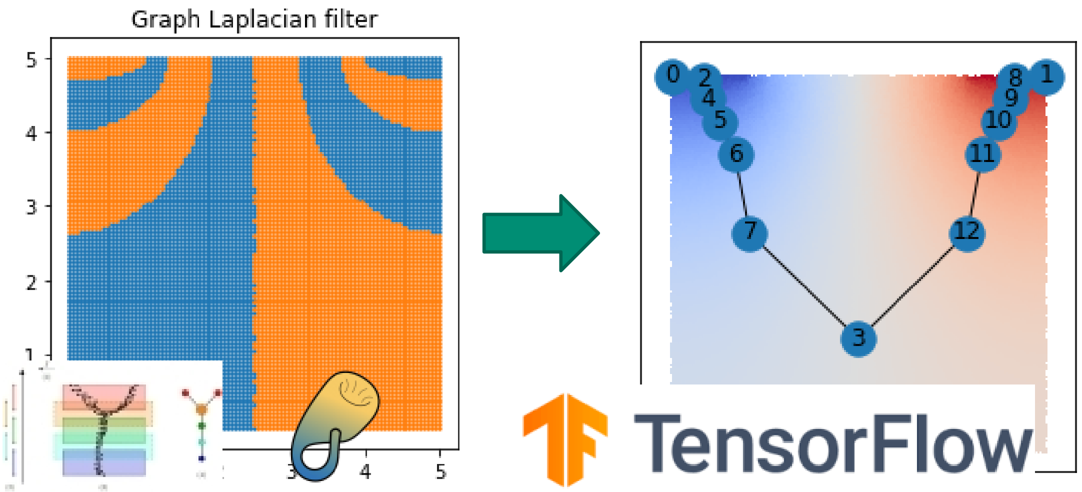
Reduced-order model from DDEC

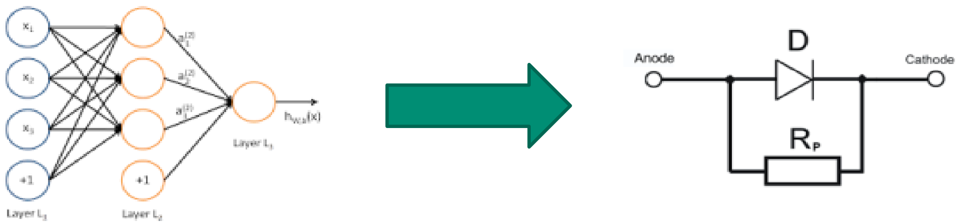
Physics-informed Graph Neural Network



Mapper & scikit-tda

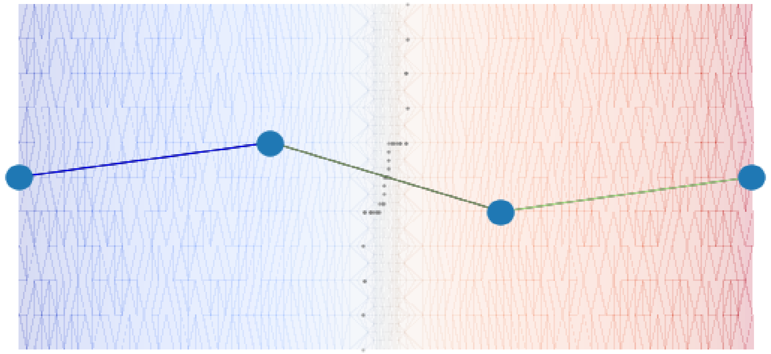
Key benefits:

- Realizes NN *computational graph topology* as a *circuit topology:*

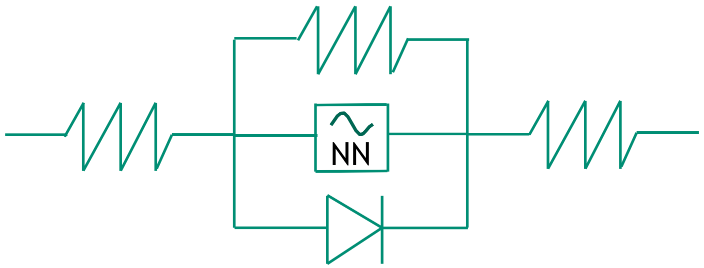


- **Transfers PDE-based physical conservation to DDEC neural network structure.**
- In contrast with state-of-the-art Physics informed Neural Networks, use PDE constraint optimization for parameter-free learning.
- Modifying PDE incorporating new physics models does not change workflow.

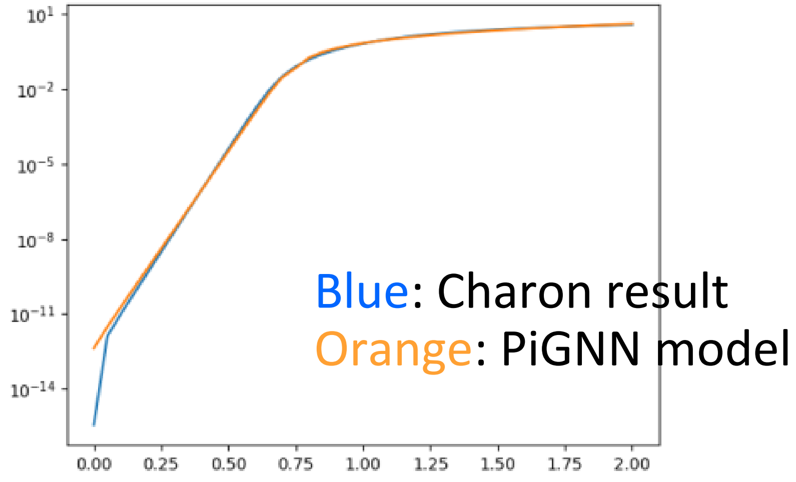
Example workflow: PN diode model on uniform partition [2]



PiGNN PN diode
compact model topology



Log(Current)-Voltage



TensorFlow learned parameters

```
edge_0-2_resistor_conductance:0 has value: 15.8
edge_1-3_resistor_conductance:0 has value: 15.8
edge_2-3_diode_I0:0 has value: 1e-13
edge_2-3_diode_knot:0 has value: 0.7641590468787397
edge_2-3_diode_exponent:0 has value: 35.91716524715814
edge_2-3_resistor_conductance:0 has value: 15.8
edge_2-3_nn_biases:0 has value: [2.46351959 ... 3.22326079]
edge_2-3_nn_weights:0 has value: [2.70549157 ... 2.29335275]
edge_2-3_nn_coeffs:0 has value: [0.53980711 ... 0.53774219]
```

Greedy Fiedler Spectral partitioning scheme

Partitioning scheme on FEM mesh

Algorithm

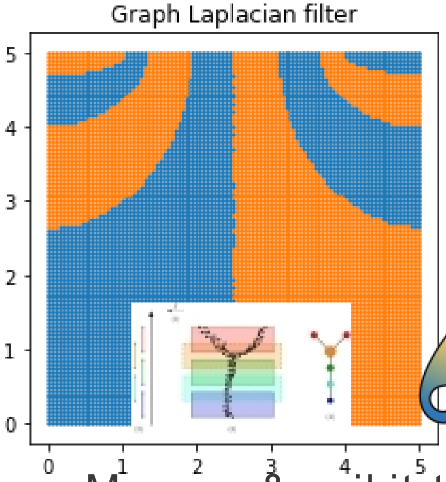
1. Obtain solution manifold (x,y, ϕ(x,y)).
Define Laplacian Δ_S on it.
Choose number of partitions N desired.

2. Compute the Fiedler eigenvector of Δ_S.
Use it to partition the domain **D**.

3. Determine partition D′ among all sub-domains
obtained with largest $L^2(\nabla\phi)$ measure.

4. Greedy

5. Constr



Mapper & scikit-tda

<u>Algorithm</u>

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2. Compute the Fiedler eigenvector of Δ_S.
   Use it to partition the domain **D**.

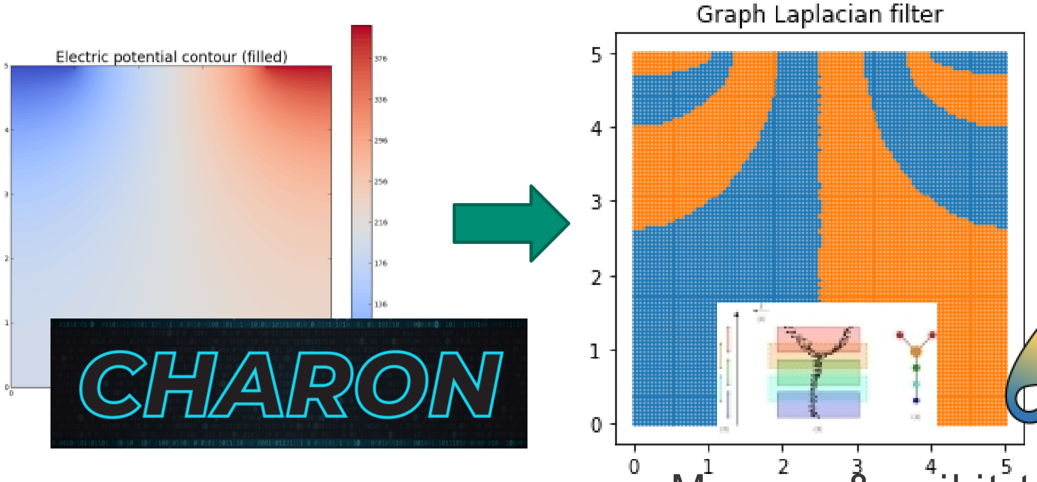
3. Determine partition **D′** among all sub-domains
   obtained with largest $L^2(\nabla\phi)$ measure.

4. Greedy step:
   If num parts < N: Go to Step 2, with **D′ → D**
   If num parts = N: Continue

5. Construct the graph **C** = $\{\{n_i\},\{e_{ij}\}\}$ *dual* to
   the domain partition.

DDEC graph from Greedy Fiedler Spectral Partitioning

Partitioning scheme on FEM mesh



Mapper & scikit-tda

<u>Key benefits:</u>

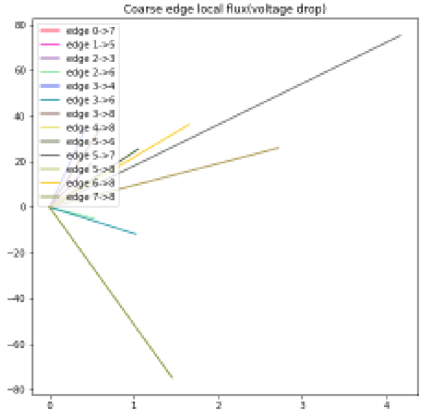
- Eigenfunctions form a basis for $\mathbf{L}^2$ functions, suggesting **well-approximability** of PDE solutions by piecewise constants on nodal sets.
- Dual graph identifies 1D flow directions, transferring structure of PDE solution dynamics to a 1D graph "backbone".

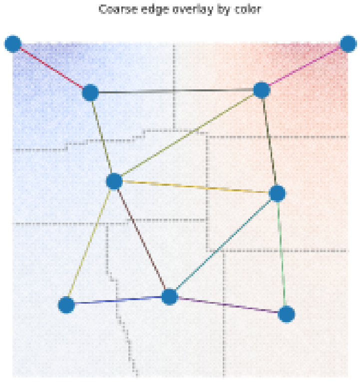
Examples: Partitioning schemes and resulting DDEC complexes

Resistor

Two contacts

Metis partition



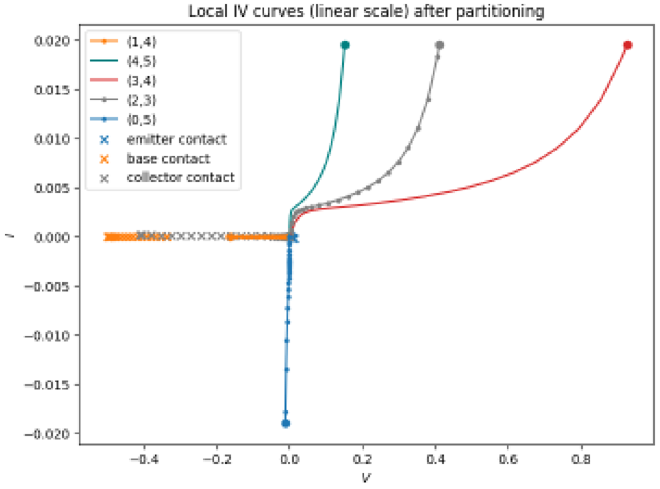


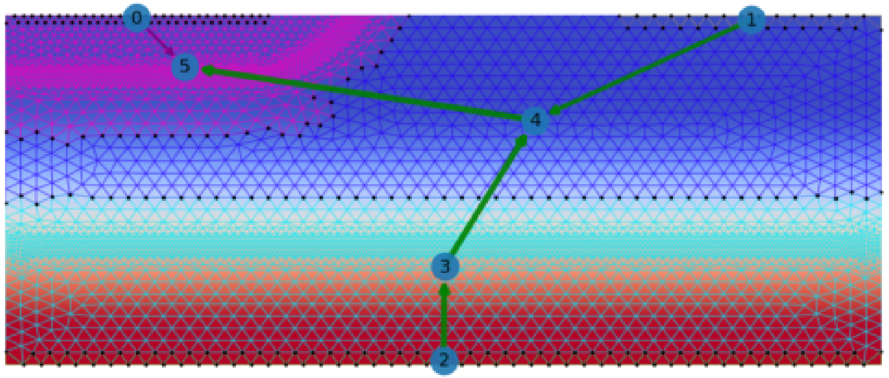
BJT (Transistor)

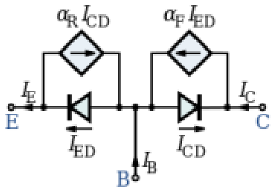
Three contacts

Eigenfunction partition

(x, y, electric potential)







Compare topology to Ebers-Moll

References

1. Enforcing exact physics in scientific machine learning: a data-driven exterior calculus on graphs
   Submitted to Journal of Computational Physics
   Preprint available: https://arxiv.org/abs/2012.11799
   Nathaniel Trask, Andy Huang, Xiaozhe Hu

2. Physics-Informed Graph Neural Network for Circuit Compact Model Development
   SISPAD International Conference on Simulation of Semiconductor Processes and Devices 2020
   doi:10.23919/SISPAD49475.2020.9241634
   Xujiao (Suzey) Gao, Andy Huang, Nathaniel Trask, Shahed Reza

3. Greedy Fiedler Spectral Partitioning for Data-driven Discrete Exterior Calculus
   AAAI Spring Series 2021 Symposium on Combining AI and ML with Physics Sciences
   Andy Huang, Nathaniel Trask, Christopher Brissette and Xiaozhe Hu

4. Partitioning Physics Data via Laplacian Nodal Sets
   SIAM CSE 2021 in two days: Thursday Mar 4 MS229 10:05-10:20 CST
   Christopher Brissette, Andy Huang and Nathaniel Trask

Software

1. BSIM model http://bsim.berkeley.edu/models/bsim4/
   VBIC model https://designers-guide.org/vbic/
2. Charon https://charon.sandia.gov/ (oper e!)
3. Xyce https://xyce.sandia.gov/ (open source!)
4. TensorFlow https://www.tensorflow.org/about/bib