Quantum Element Method for Multi-Dimensional Nanostructures Enabled by a Projection-based Learning Algorithm

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Clarkson™

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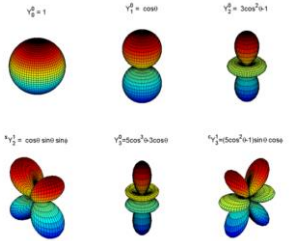
NANOSTRUCTURES

- Useful applications in medicine, chemistry and material science
- Often with nanostructures one needs to work with the Schrödinger equation

$$\nabla \cdot \frac{-\hbar^2}{2m^*(\vec{r})} \nabla\psi(\vec{r}) + U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

- Large-scale multi-dimensional simulations of the Schrödinger equation often require immense computational power and time when using direct numeric simulations (DNS)
  - Like many other special dependent simulations, a large number of DoF are needed, especially in regions where high resolution is needed

ESSENTIALS OF COMPACT MODELING



- Employ projection or Mathematical Transformation to reduce the DoF
  - Commonly used projections:
    - Fourier Series: $f(x) = \sum_{-\infty}^{\infty} a_n e^{jnkx}$: Periodic Harmonic Expansion
    - Legendre Polynomials: $f(x) = \sum_{\ell=0}^{n} a_\ell P_\ell(x)$: Spherical Harmonic Expansion
    - Bessel Functions: $f(x) = \sum_{n=0}^{M} a_n J_{n(x)}$: Cylindric Harmonic Expansion
  - Instead of assuming a basis, a learning algorithm can extract the modes:
  - Examples:
    - PCA: Principal component analysis
    - SVD: Singular value decomposition

- Spherical Harmonic

https://www.theochem.ru.nl/~pwormer/Knowino/knowino.org/wiki/Spherical_harmonics.html

Proper Orthogonal Decomposition of The Schrödinger Eqn.

- To reduce DoF of the Schrödinger equation one will project it onto modes found via POD

$$\psi(\vec{r}) = \sum_{i=1}^{M} a_i \eta_i(\vec{r})$$

- POD modes $\eta(\vec{r})$ are found such that it maximizes its mean square inner product with the solution

$$\left\langle \left(\int_{\Omega} \psi(\vec{r})\, \eta(\vec{r}) d\Omega \right)^2 \right\rangle \Big/ \int_{\Omega} \eta(\vec{r})^2 \, d\Omega$$

- Employing Calculus of variations techniques, the maximization process results in an eigenvalue problem of the 2-point correlation matrix of the data

$$\int_{\Omega'} \langle \psi(\vec{r}) \otimes \psi(\vec{r'}) \rangle \eta(\vec{r'}) d\Omega' = \lambda \eta(\vec{r})$$

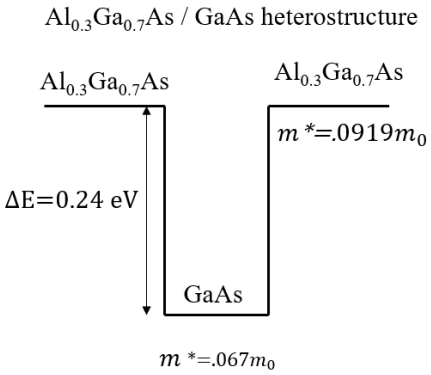
- Solved modes minimize the least square error with the smallest number of basis functions

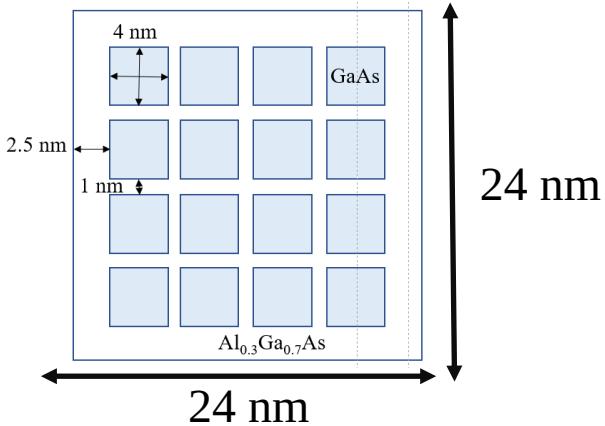
QUANTUM POD METHODOLOGY FOR SINGLE ELEMENT

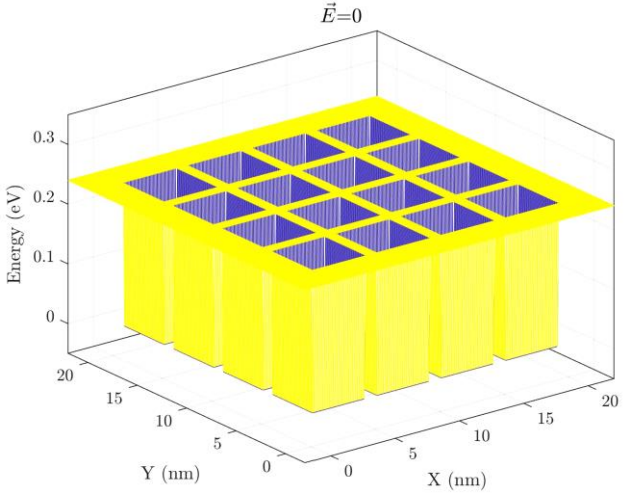
- Data collected via applying electric fields or external potentials to underlining nanostructure
- For each sample (applied electric field) the Schrödinger Eqn. is solved using DNS
- WFs of the first few N QS are collected for N_s electric fields

Ψ_i : Set of WF data for Electric field i

$$Total\ Data = \{\Psi_1, \Psi_2, \dots, \Psi_{N_S}\}; \Psi_i = \{\psi_1(\vec{r}), \psi_2(\vec{r}), \dots, \psi_N(\vec{r})\}$$







Single Element Projection onto POD Modes

Schrodinger equation formed via a linear combination of POD Modes:

$$\psi(\vec{r}) = \sum_{i=1}^{M} a_i \eta_i(\vec{r})$$

Galerkin Projection of the Schrodinger equation onto the ith POD mode:

$$\int_\Omega \nabla\eta_i \cdot \frac{\hbar^2}{2m^*}\nabla\psi d\Omega + \int_\Omega \eta_i U\psi d\Omega - \int_S \eta_i \frac{\hbar^2}{2m^*}\nabla\psi \cdot d\vec{S} = E\int_\Omega \eta_i\psi d\Omega$$

Unlike PCA/SVD, the POD simulation methodology involves a second projection incorporating the governing equation into the model

Forms Hamiltonian Equation in POD Space: $\boldsymbol{H}_\eta\vec{a} = \left(\boldsymbol{T}_\eta + \boldsymbol{B}_\eta + \boldsymbol{U}_\eta\right)\vec{a} = \mathrm{E}\vec{a}$

$$\boldsymbol{T}_{\eta i,j} = \int_\Omega \left[\nabla\eta_i(\vec{r}) \cdot \frac{\hbar^2}{2m^*}\nabla\eta_j(\vec{r})\right] d\Omega$$

Interior kinetic energy matrix

$$\boldsymbol{B}_{\eta i,j} = -\int_S \eta_i(\vec{r}) \frac{\hbar^2}{2m^*}\nabla\eta_j(\vec{r}) dS$$

Boundary kinetic energy matrix

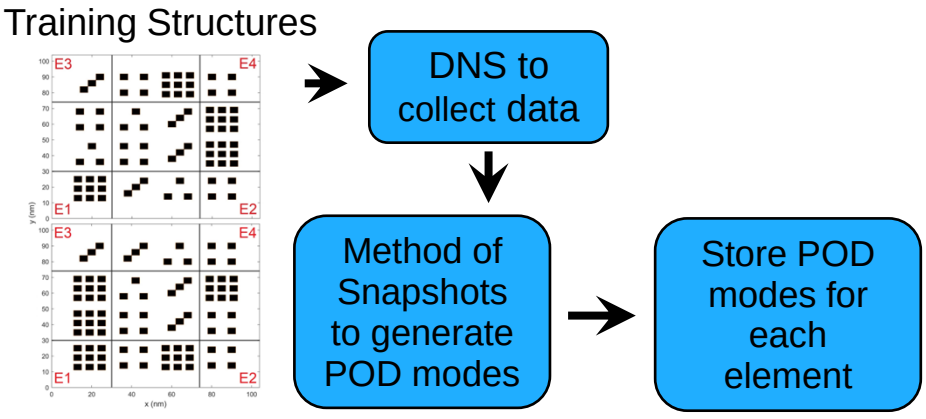
$$\boldsymbol{U}_{\eta i,j} = \int_\Omega \eta_i(\vec{r}) U(\vec{r}) \eta_j(\vec{r}) d\Omega$$

Potential energy matrix

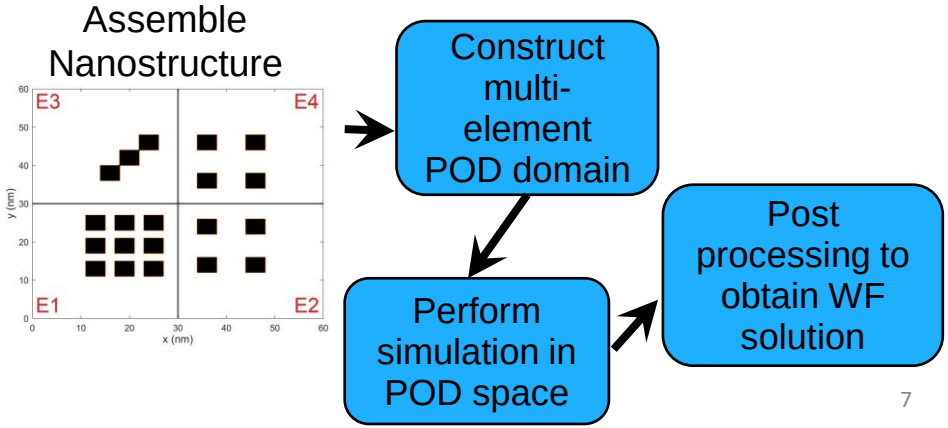
Quantum Element Method (QEM)

- To form the POD modes, DNS data is required
  - Large structures might make gathering this training data prohibitive due to large simulation times.
- Solution: QEM
  - Incorporate domain decomposition in which trained elements can be stitched using the Discontinuous Galerkin Method
  - Aligning with the engineering paradigm of building Blocks the QEM offers a cost-effective approach to simulating large nanostructures

Train Elements



Application



SCHRODINGER EQUATION, IN POD SPACE (QEM)

$$\int_{\Omega} \nabla\eta_i \cdot \frac{\hbar^2}{2m^*} \nabla\psi d\Omega + \int_{\Omega} \eta_i U\psi d\Omega - \int_{S} \eta_i \frac{\hbar^2}{2m^*} \nabla\psi \cdot d\vec{S} = E \int_{\Omega} \eta_i \psi d\Omega$$

- Applying the Discontinuous Galerkin method to the Schrodinger equation in POD space the results in:

$$\sum_{j=1}^{M_p} \left(T_{\eta_p,ij} + U_{\eta_p,ij}\right) a_{p,j} + \sum_{q=1,q\neq p}^{Nel} \sum_{j=1}^{M_p} B_{p,pq,ij} a_{p,j} + \sum_{q=1,q\neq p}^{Nel} \sum_{j=1}^{M_p} B_{pq,ij} a_{p,j} = E a_{p,i}$$

Interior Kinetic energy Matrix

Interior Potential energy Matrix

μ penalty parameter allowing control preference between continuity of flux vs value

$$B_{p,pq,ij} = -\frac{1}{2} \int_{\Omega_p} \frac{\hbar^2}{2m_p^*} \left[(\nabla\eta_{p,i})\eta_{p,j} + \eta_{p,i}(\nabla\eta_{p,j})\right] \cdot d\vec{S} + \mu \int_{S_{pq}} \frac{\hbar^2}{2m_p^*} \eta_{p,i}\, \eta_{p,j} dS$$

Diagonal Boundary Kinetic Energy Matrix

$$B_{pq,ij} = \frac{1}{2} \int_{\Omega_p} \frac{\hbar^2}{2m_p^*} \left[(\nabla\eta_{p,i})\eta_{q,j} + \eta_{p,i}(\nabla\eta_{q,j})\right] \cdot d\vec{S} - \mu \int_{S_{pq}} \frac{\hbar^2}{2m_p^*} \eta_{p,i}\, \eta_{q,j} dS$$

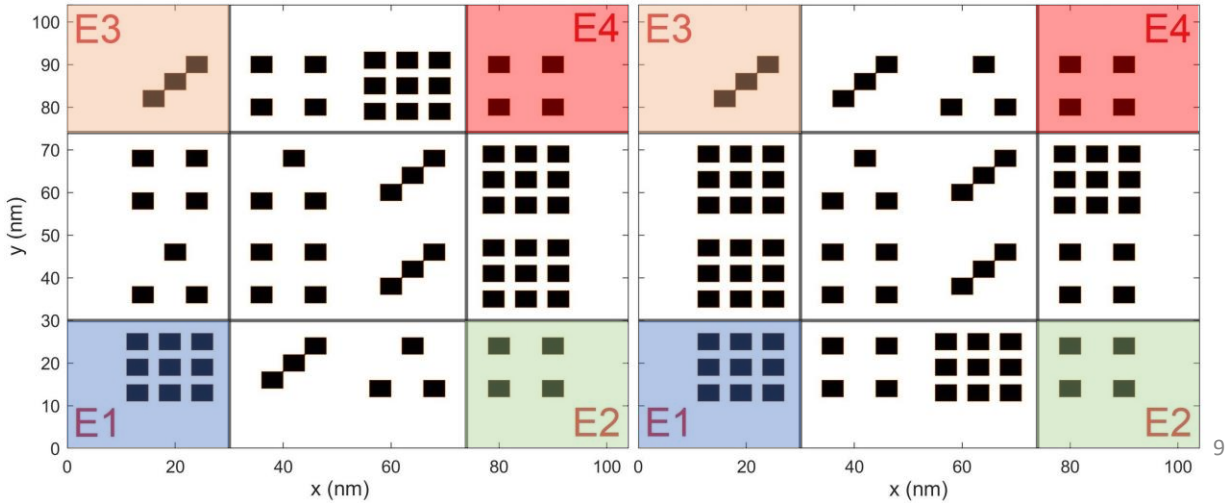
Off-Diagonal Boundary Kinetic Energy Matrix

Training and Mode Generation

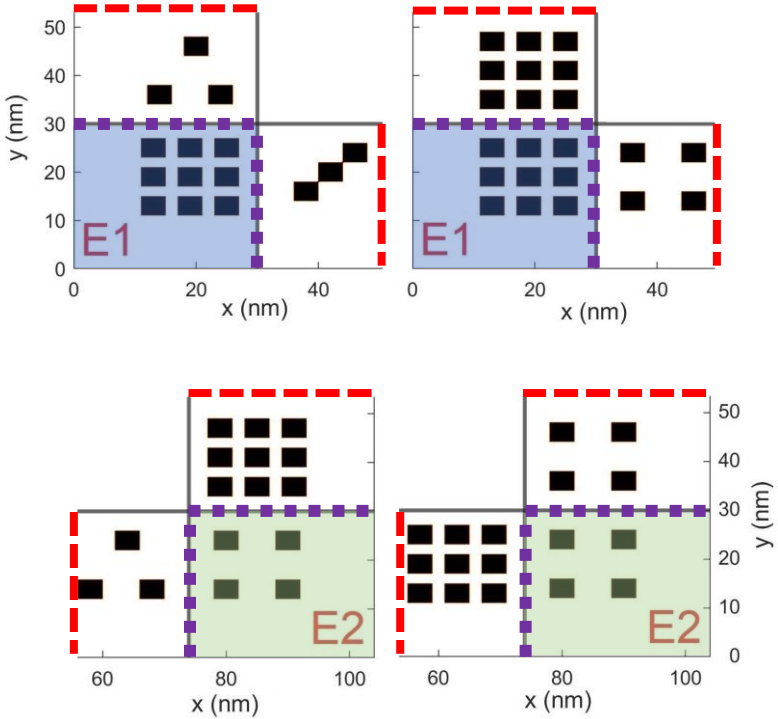
- Two 9-element training structures of quantum dots composed of the GaAs/InAs heterostructure are for training
  - 5 electric field applied in each of the two orthogonal directions ranging from -0.35kv/cm and +0.35kv/cm are applied to these structures.
  - For each Electric Field, the WFs of the first 6 QSs are collected.

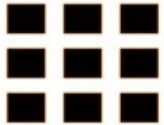
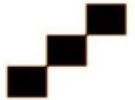
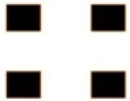
- After Training

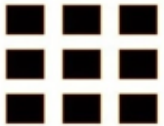
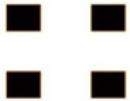
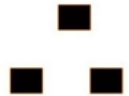
the POD modes, the Method of Snapshots
is applied to each element generating a unique set of Modes for each.



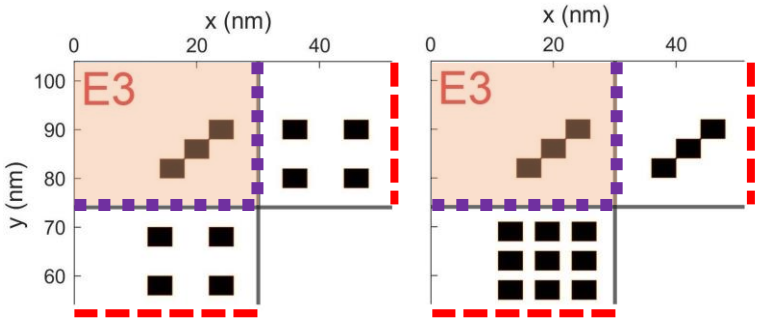
Training Elements 1and 2

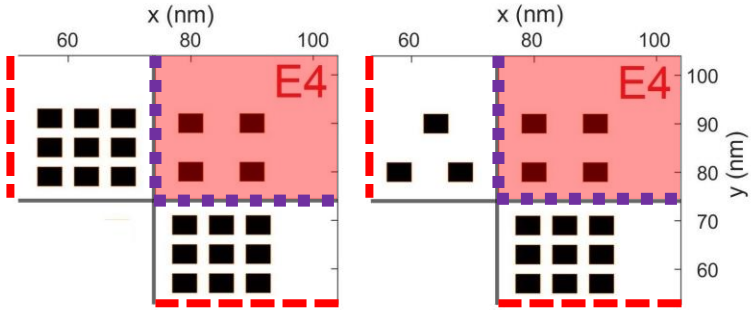


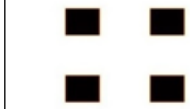
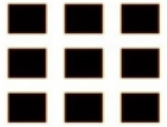
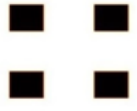
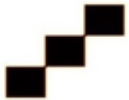
Vertical Training Elements		
Horizontal Training Elements		

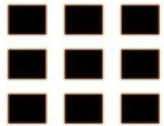
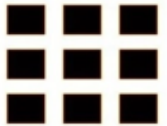
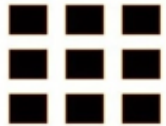
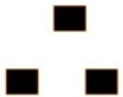
Vertical Training Elements		
Horizontal Training Elements		

Training Element 3 and 4





Vertical Training Elements		
Horizontal Training Elements		

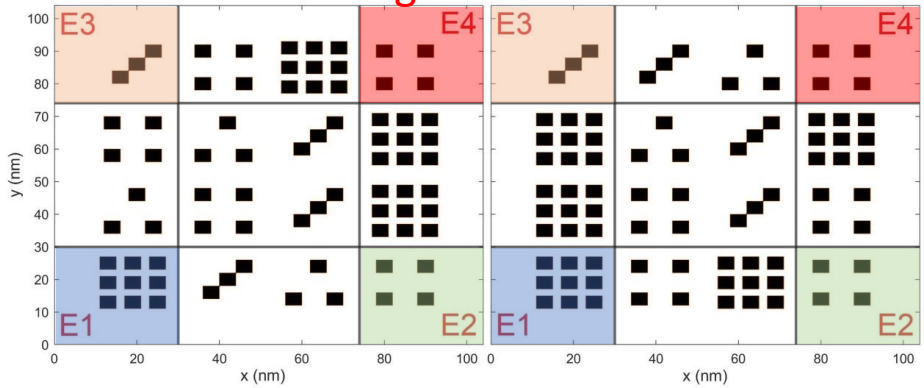
Vertical Training Elements		
Horizontal Training Elements		

TEST STRUCTURE

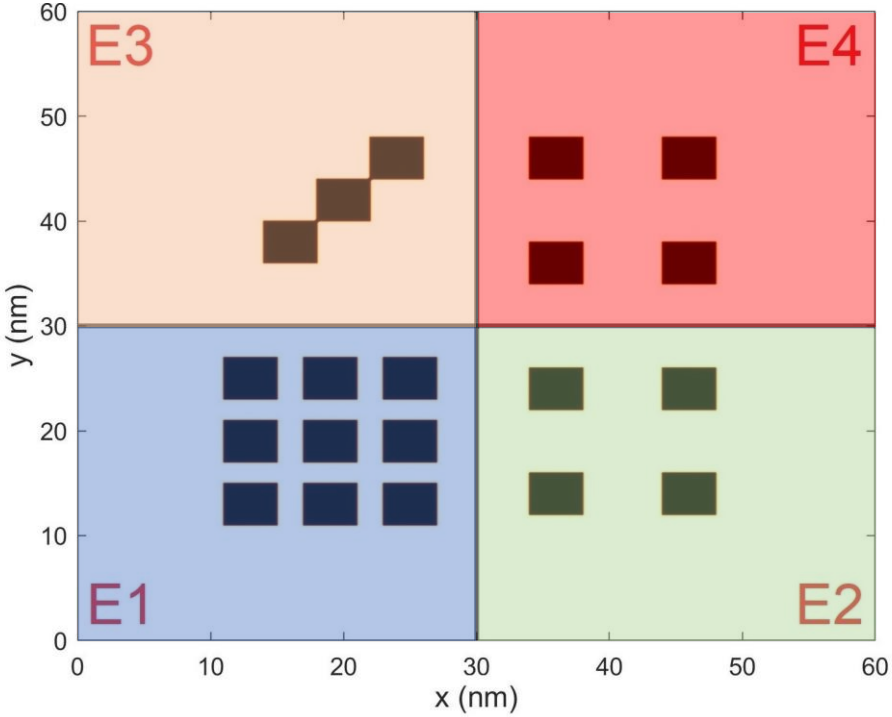
- The POD methodology is applied to the training structure on right.
- Unlike during training, a two-component electric field is applied

$$\vec{E} = 25\frac{kV}{cm}\hat{x} - 15\frac{kV}{cm}\hat{y}$$

Training Nanostructure

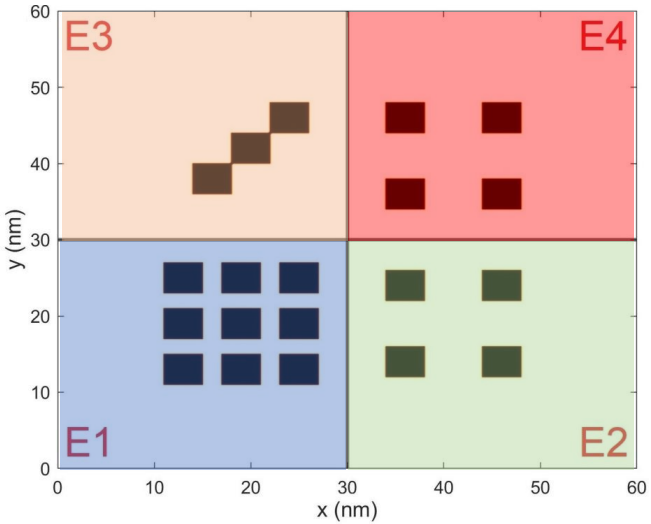


Test Nanostructure



Adequacy of Training relative to test Structure

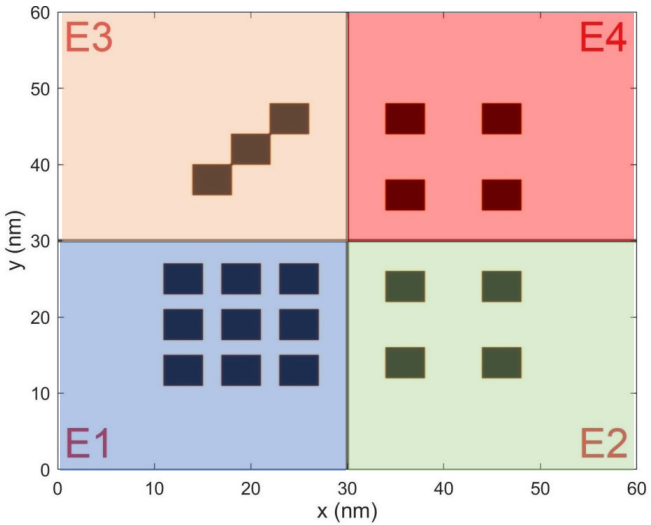
Test Nanostructure



	Training Elements		Test	
Vertical E1				✗
Horizontal E1				✓
Vertical E2				✓
Horizontal E2				✓

Adequacy of Training relative to test Structure Cont.

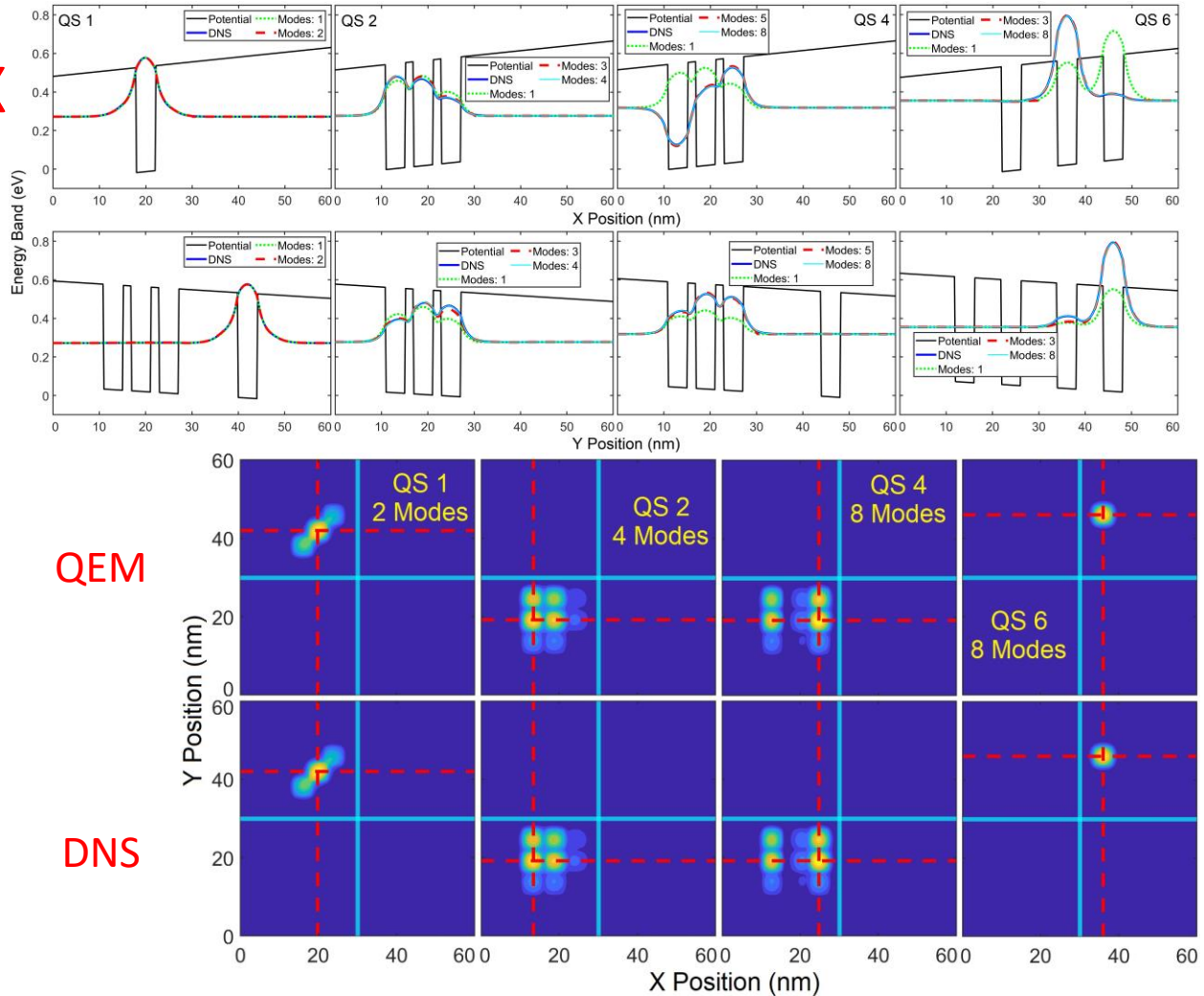
Test Nanostructure



	Training Elements		Test	
Vertical E3				✓
Horizontal E3				✓
Vertical E4				✘
Horizontal E4				✘

ψ RESULTS

- Alignment with POD and DNS solution after around 10 modes per Element



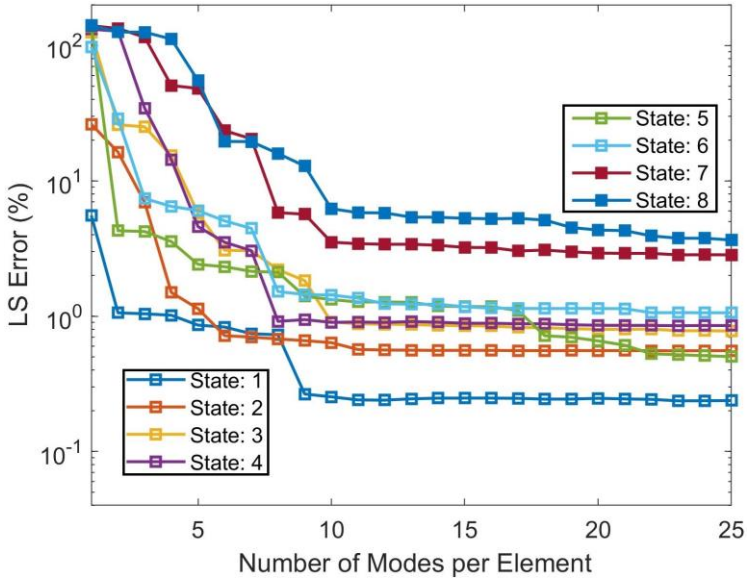
LS Error Plot and Energy Error

Tab. 1. Percentage Error of Eigenenergy in Each State

QS	POD Energy (eV)	DSN Energy (eV)	(%) Difference
1	0.29888	0.29701	0.62631
2	0.30360	0.30229	0.43295
3	0.34313	0.34119	0.56768
4	0.34545	0.34354	0.55297
5	0.35336	0.35097	0.67970
6	0.38199	0.37969	0.60448
7	0.38521	0.38263	0.67287
8	0.39698	0.39371	0.82581

- Energy Percent difference between DNS and POD is less than 0.7% for trained states and 0.83% for untrained states

DNS uses 90601 DoF



- LS error for trained states is around 1% or less after including 10 modes for trained states.
- States 7 and 8 which are not trained reach an errors or around 3% and 4% respectively after including 20 Modes per element.

CONCLUSION

- QEM can greatly reduce the DoF of the problem
  - 90601 to around 40 DoF
- QEM confirms the engineering paradigm of building blocks
  - Offers promising value within engineering design
- In general, higher QSs require more POD modes to reach sufficient accuracy
- The QEM can stitch together blocks with incomplete training
- Training with single orthogonal component electric fields allows simulation of nanostructures subjected to two components
- Higher untrained QSs can be reasonably predicted via the QEM
- For large Nanostructures, the POD Hamiltonian matrix becomes sparse