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SAND2015-1300C

Device-Level Models Using Multi-Valley Effective Mass

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Collaborators and Nomenclature

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- **Collaborators:**
  - John King Gamble → G37.00007, full-scope modeling
  - Toby Jacobson → W37.00009, open dynamics
  - Adam Frees → W37.00010, donor-dot tunneling
  - Everyone else → Xujiao (Suzey) Gao, John Mitchell, Inès Montaño, Rick Muller, and Erik Nielsen
- **Nomenclature:**
  - 2DEG → Two-Dimensional Electron Gas
  - CI → Configuration Interaction
  - DG → Discontinuous Galerkin
  - DQD → Double Quantum Dot
  - EMT → Effective Mass Theory
  - FEM → Finite Element Method
  - PDE → Partial Differential Equation
  - QCAD → Quantum Computer Aided Design
  - VO → Valley-Orbit

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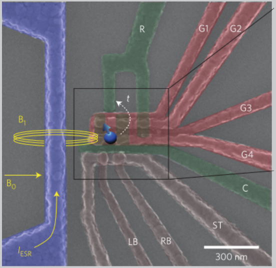
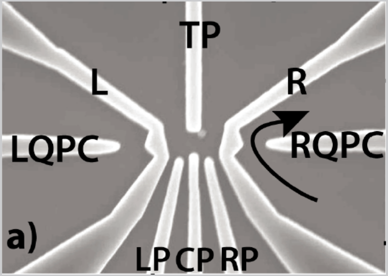
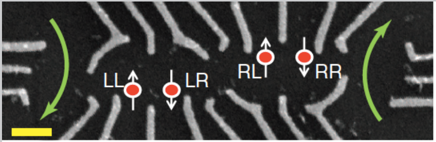
Motivation



Veldhorst, et. al., *Nature Nano* (2014)



Nguyen, et. al., arXiv:1403.3704



Shulman, et. al., *Science* (2012)

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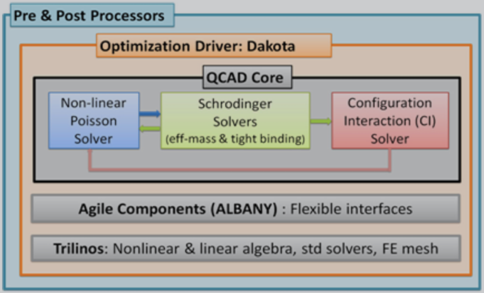
- SNL's self-consistent electrostatics / quantum package
- FEM discretization of PDEs
- See Gao, Nielsen, et. al., *J. App. Phys.*, 2013



- **Currently:** strictly electrostatics, standard effective mass, and full-CI
- **Goal:** add physics to achieve high-fidelity model of qubit/environment
- **Problem:** more physics → complex solvers → high accuracy in solution

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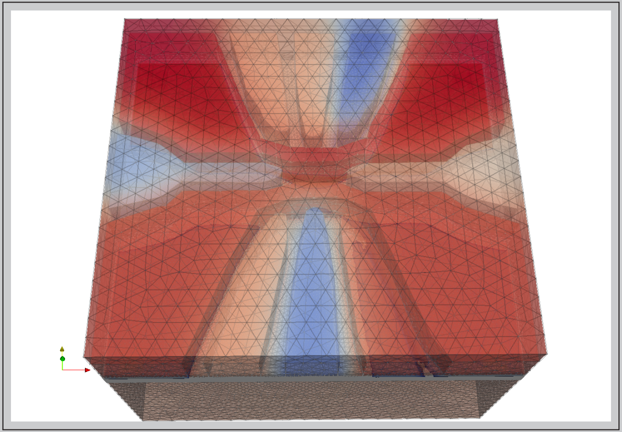
Effective Mass as a Multi-scale Problem



Red $\rightarrow$ positive potential, blue $\rightarrow$ negative potential
Domain size $\sim$ 1.5 microns

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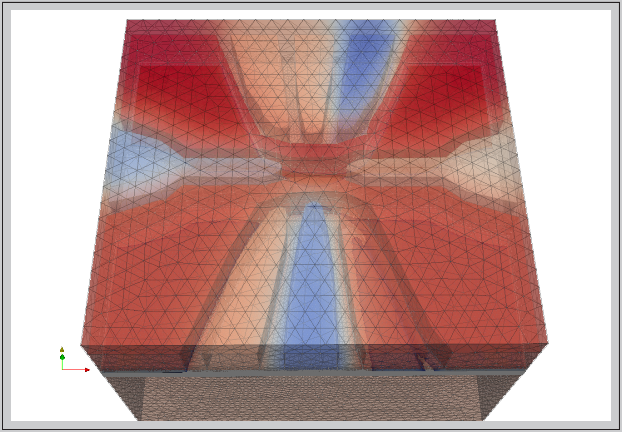

Largest edge length in gates $\sim$ 75 nanometers

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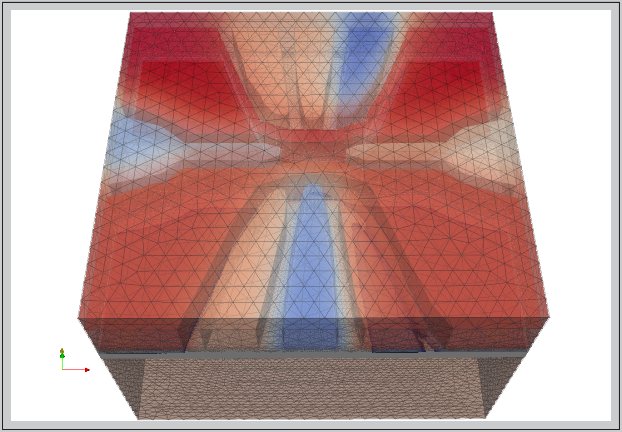

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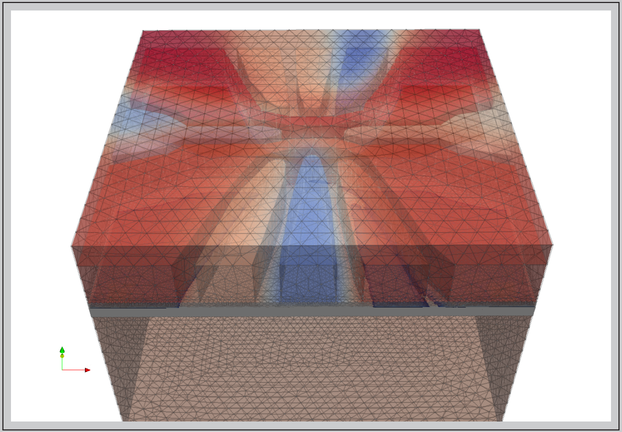

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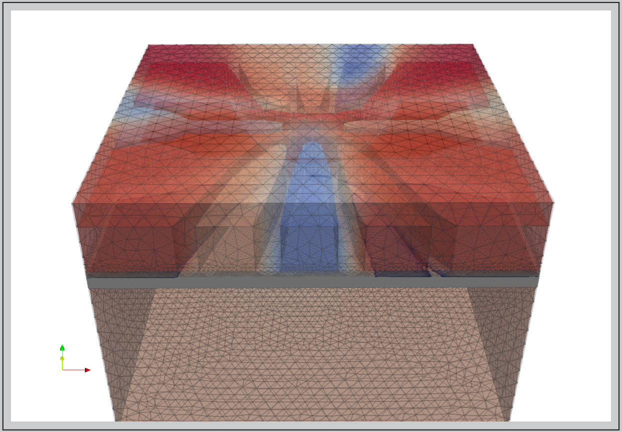

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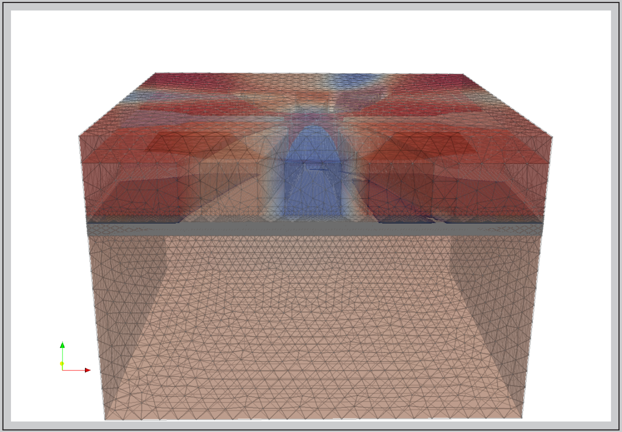

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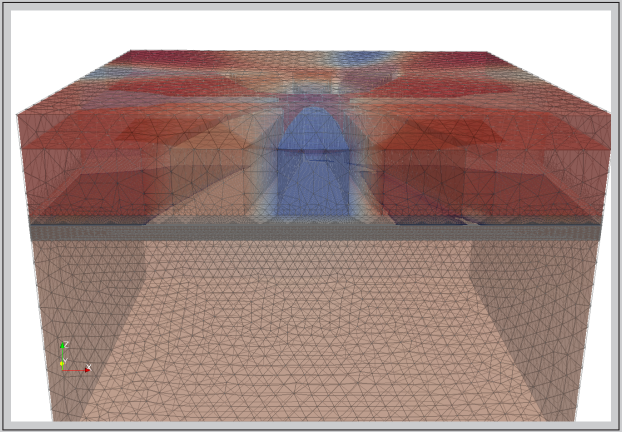

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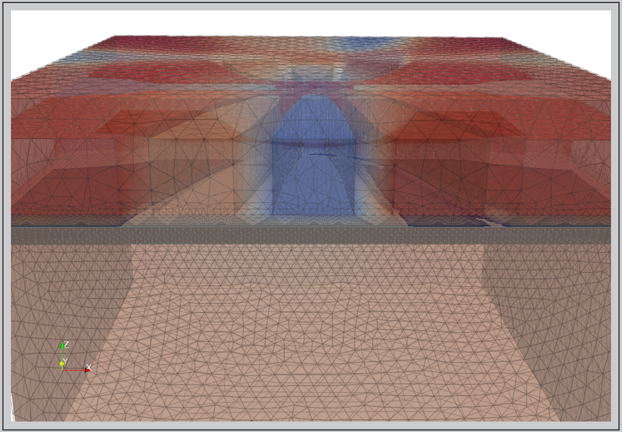

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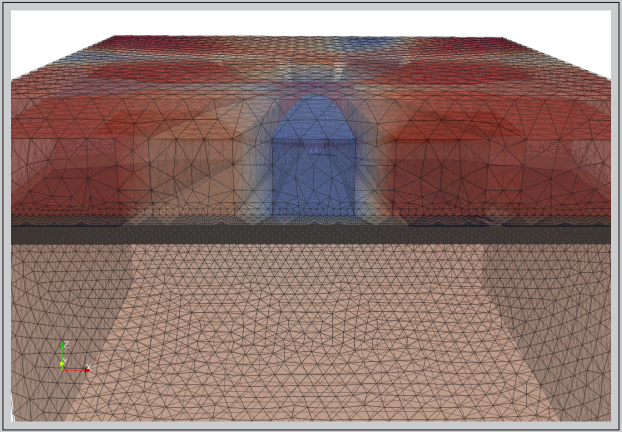

Approaching the 2DEG transition to $\sim$ 20 nanometers

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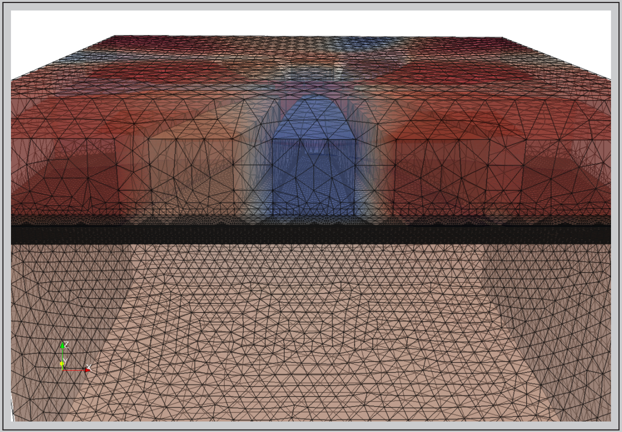

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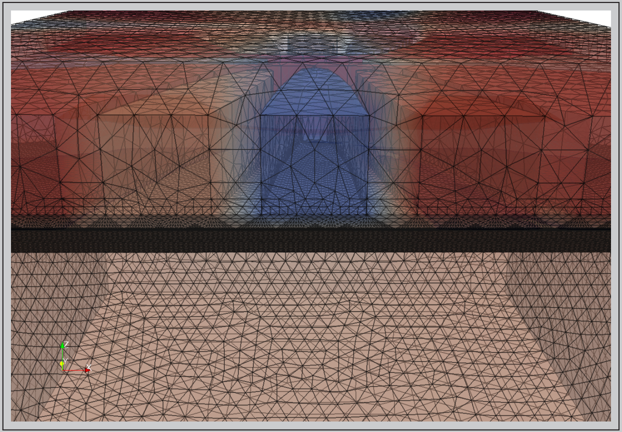

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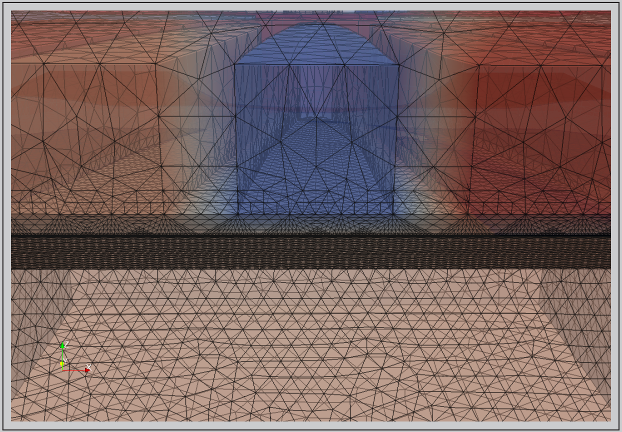

Approaching the 2DEG transition to $\sim$ 20 nanometers

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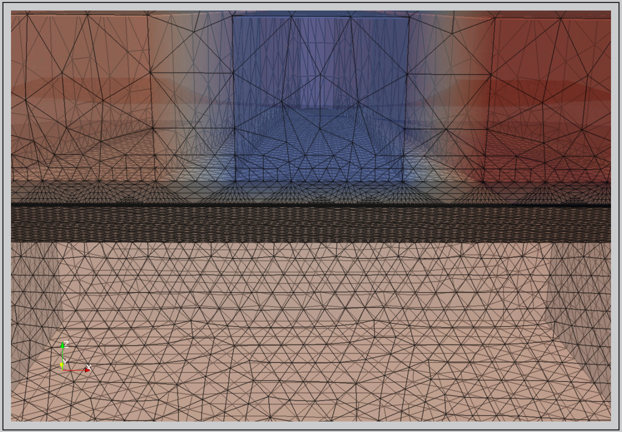
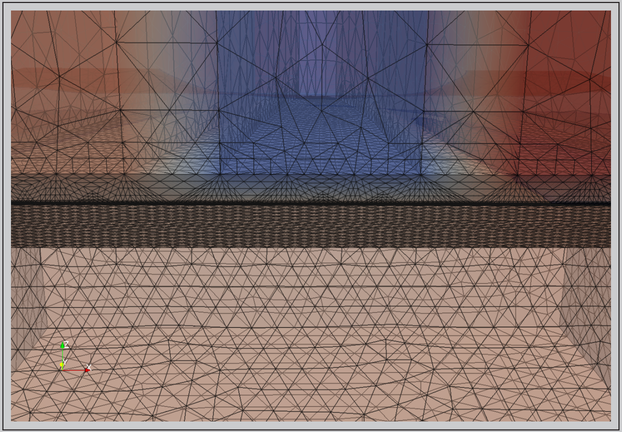


Down to $\sim$ 5 nanometers



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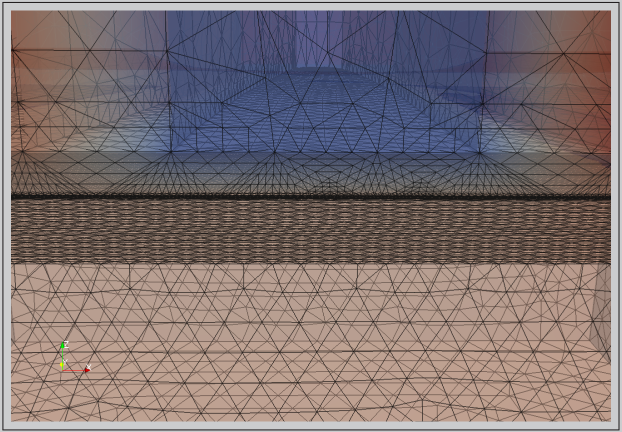

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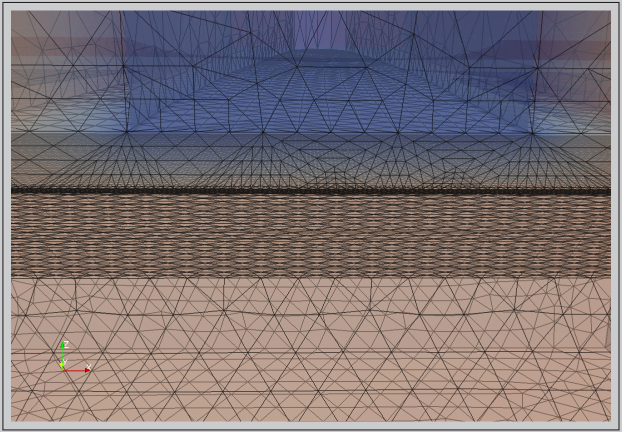

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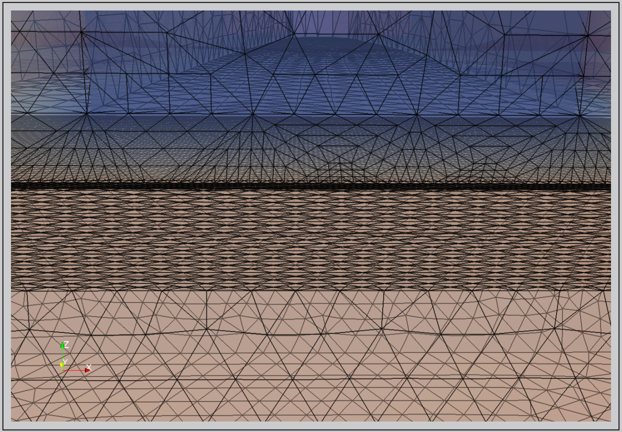

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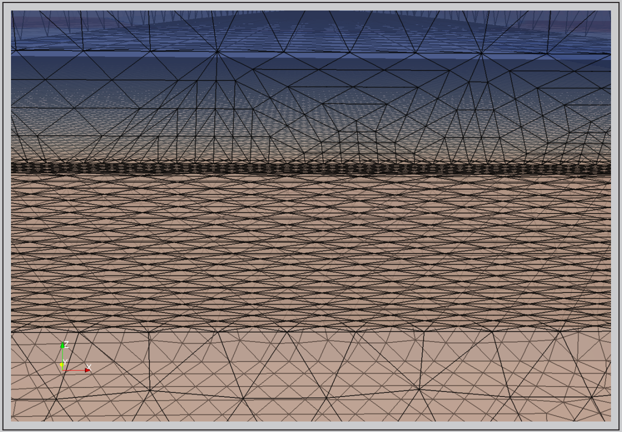

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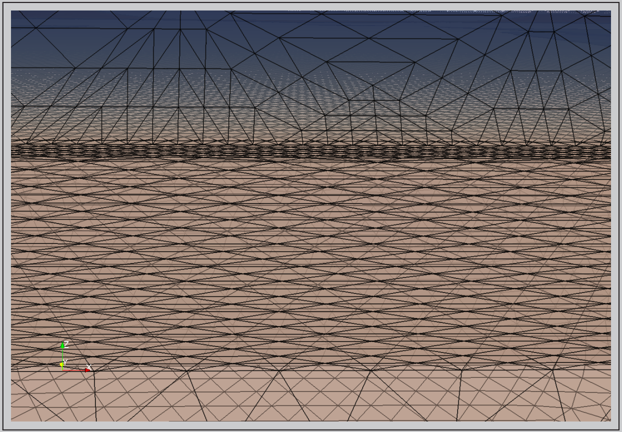

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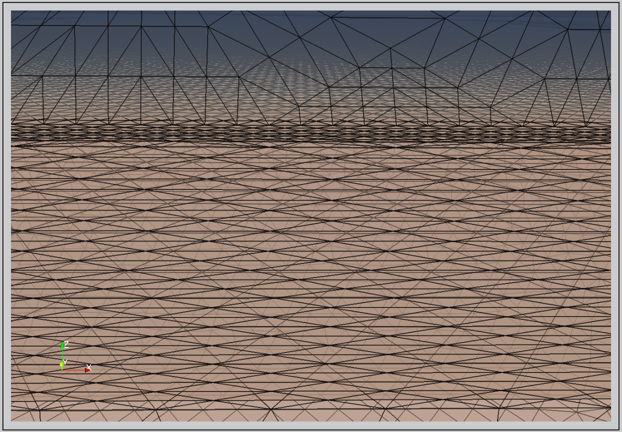
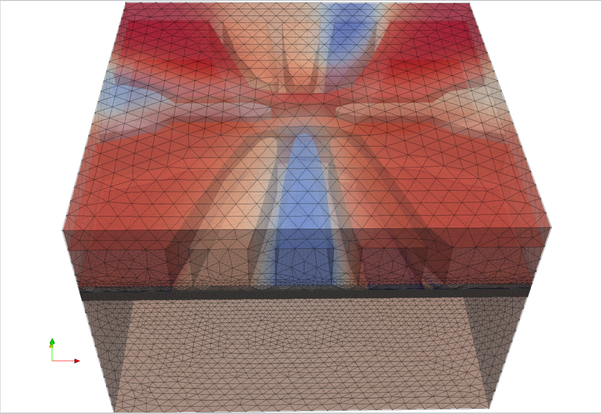


At the shortest scale is $\sim$ 1 nanometer

Effective Mass as a Multi-scale Problem



Looking at potential, level of refinement seems excessive…

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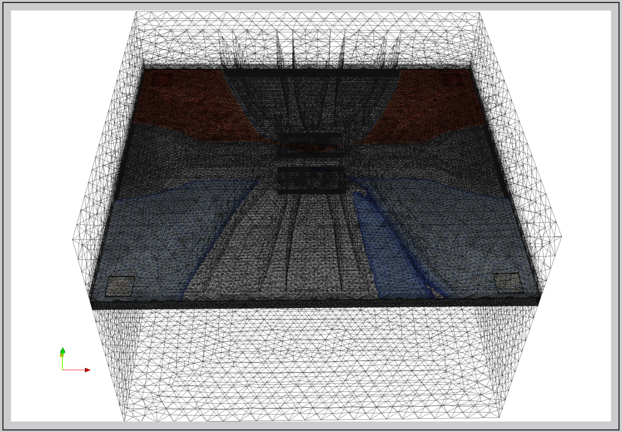
Effective Mass as a Multi-scale Problem



Looking at the electron density, we see why it is needed. . .

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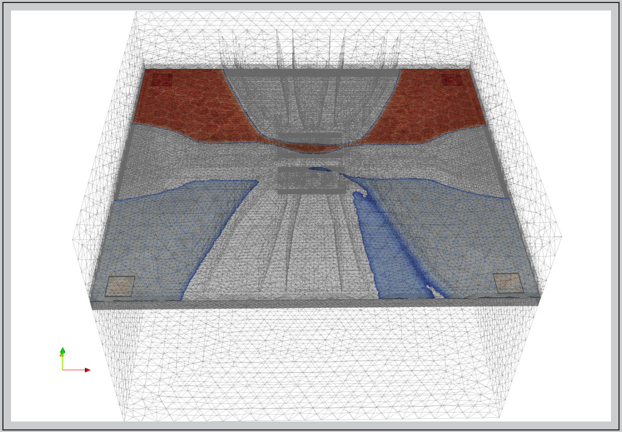

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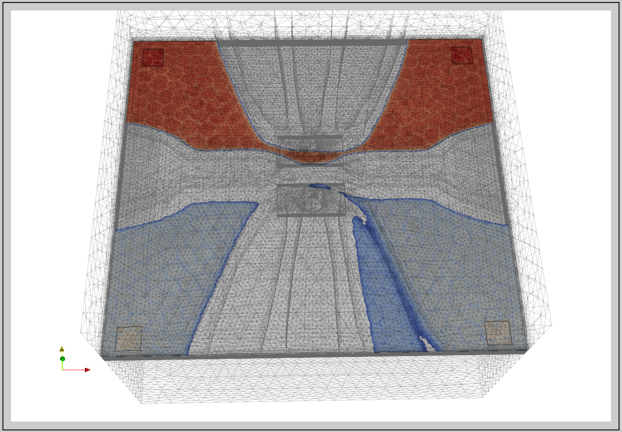

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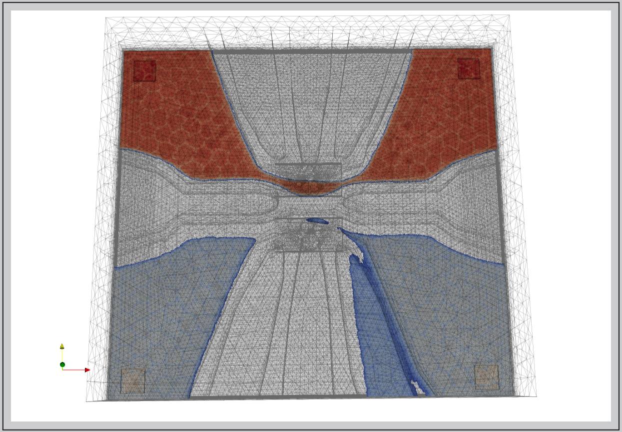

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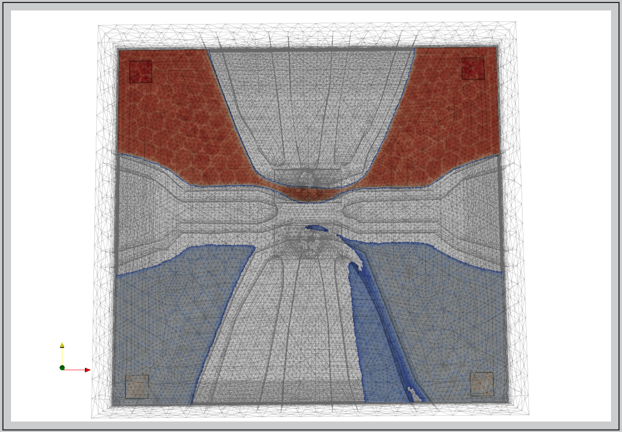

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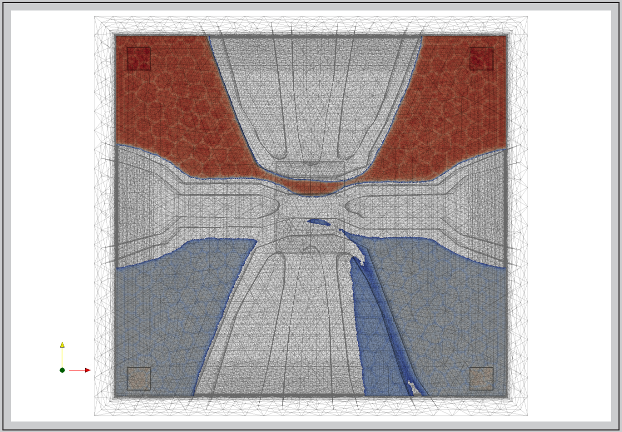

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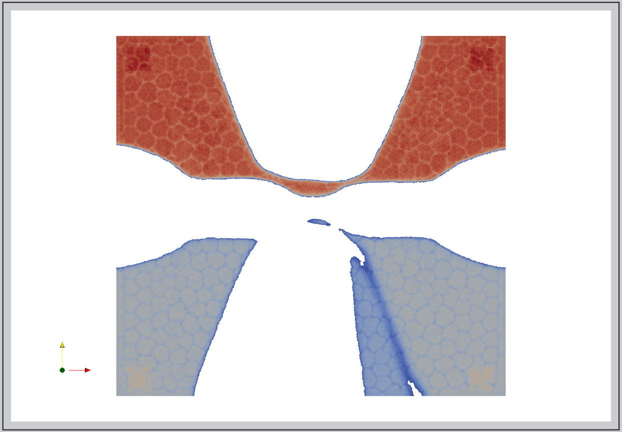

For a DQD device we need to resolve this 2DEG, working with donors/interfaces we need to go the Angstrom scale

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Multi-valley Effective Mass: Overview

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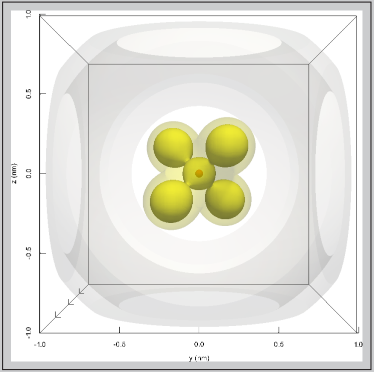
- Angstrom-level physics included in multi-valley effective mass
- Recent work, Gamble/Jacobson, et. al. - **arXiv:1408.3159**
  - Tetrahedral central cell
  - Anisotropic Gaussian basis
  - First principles Bloch functions



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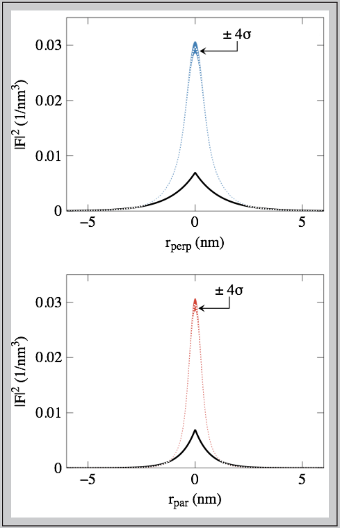

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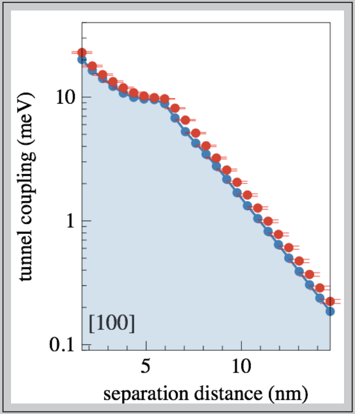

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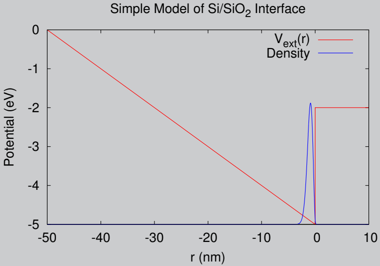
Multi-valley Effective Mass: Challenges

- Surprisingly difficult PDE: multi-scale, oscillatory coefficients

$$\left(-\frac{\hbar^2}{2}\nabla\cdot\overline{\overline{m}}(\mathbf{r})^{-1}\cdot\nabla+V_{ext}(\mathbf{r})\right)F_j(\mathbf{r})+\sum_{k\neq j}V_{jk}^{VO}(\mathbf{r})F_k(\mathbf{r})=EF_j(\mathbf{r})$$

$$V_{jk}^{VO}(\mathbf{r})=\phi_j^*(\mathbf{r})\phi_k^*(\mathbf{r})V_{ext}(\mathbf{r})$$



1D multi-valley EMT at interface inspired by Saraiva, et. al., PRB (2011)

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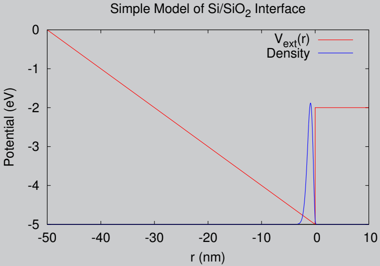

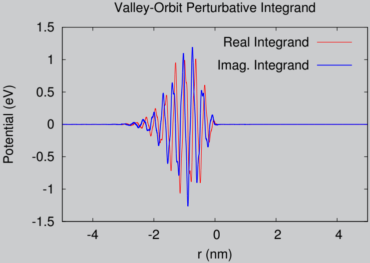

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- **Goals:**
  - Systematically improvable numerical method
  - Efficient embedding into QCAD-like framework
  - Amenable to interfacing with atomistics

What can we learn from engineers/applied mathematicians to solve difficult PDE-based models?

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Crash Course in Basis Sets

- Problems with resolution arise from incomplete use of known physics

"Physicist's" variational basis	**"Engineer's" approach (e.g., FEM)**
Perturbation on solved problem	Agnostic of problem instance
Gaussians, Sturm-Liouville eigenfunctions, etc.	Local polynomials, samples + stencil, etc.
Global support $\to$ dense	Compact support $\to$ sparse
Difficult to adapt	Natural adapativity
Few degrees of freedom	Many degrees of freedom
Boundary conditions**?**	Boundary conditions**!**

- **Features of both needed for full-scope/multi-scale problems**

Discontinuous Galerkin framework allows us to stitch together optimal solutions

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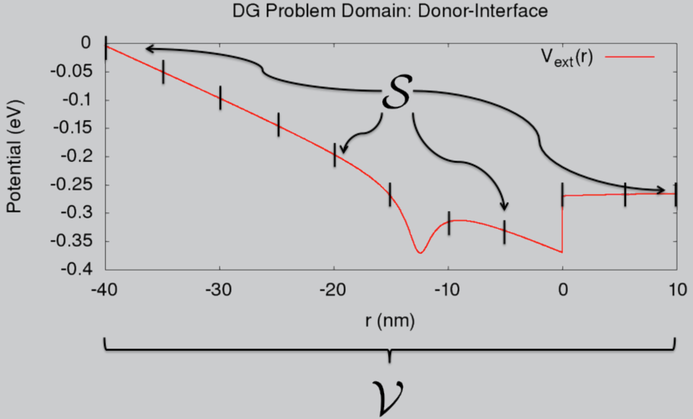
1. Break **domain** ($\mathcal{V}$) into **sub-domains** with a set of **interfaces** ($\mathcal{S}$)
2. Choose basis ($\{u_{j,k}\}$) for sub-domain k based upon **local physics**
3. **Weak soln.** of Schrödinger eqn. $\rightarrow$ soln. of **variational problem**



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DG: Step-by-Step

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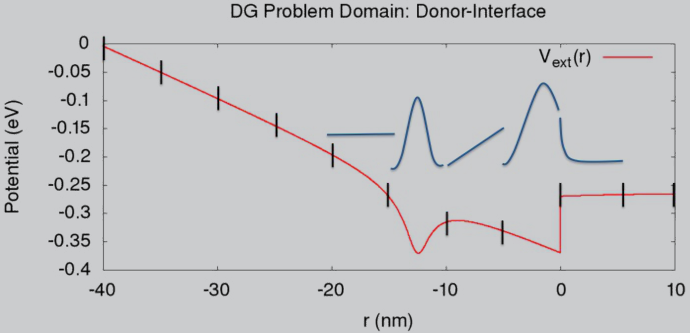

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Minimize $\mathcal{E}\left[\psi_i\right]$ for $\psi_i \in \text{span}\{u_{j,k}\}$ $\rightarrow$ Euler-Lagrange looks like Schrödinger

$$\mathcal{E}\left[\psi_i\right] = \frac{1}{2}\langle \nabla u_{j,k}, \nabla \psi_i \rangle_{\mathcal{V}} - \frac{1}{2}\langle \{\{\nabla u_{j,k}\}\}, [[\psi_i]] \rangle_{\mathcal{S}} - \frac{1}{2}\langle [[u_{j,k}]], \{\{\nabla \psi_i\}\} \rangle_{\mathcal{S}}$$
$$+ \frac{\alpha}{h}\langle [[u_{j,k}]], [[\psi_i]] \rangle_{\mathcal{S}} \langle u_{j,k}, V_{ext}\psi_i \rangle_{\mathcal{V}} = E_i \langle u_{j,k}, \psi_i \rangle_{\mathcal{V}}$$

- FEM: arbitrary element of span$\{u_{j,k}\}$ is continuous
- DG: arbitrary element is discontinuous $\rightarrow$ $\mathcal{E}\left[\psi_i\right]$ finds "continuous" ones

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DG: Simple Example

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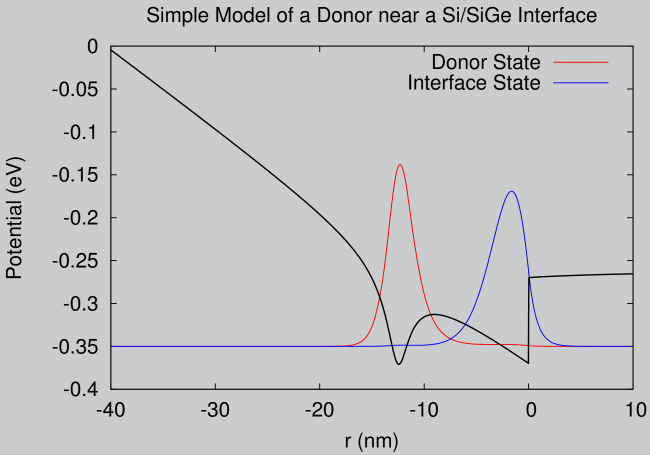
Solving for envelope states of interest:



60 unknowns $\rightarrow$ ground state and VO coupling to $\sim$ 0.01%

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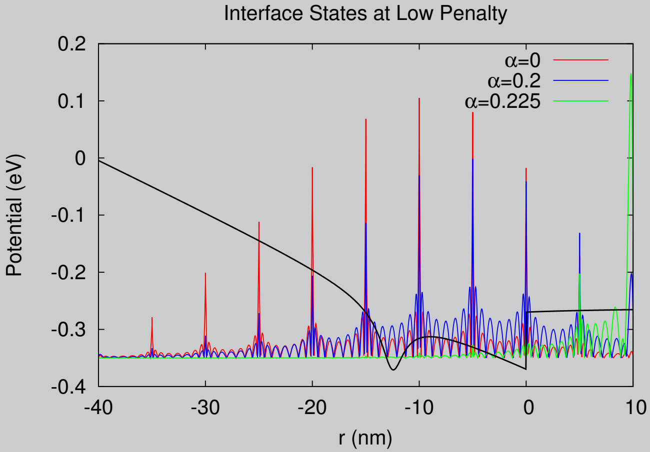
α parameter pushes pathological solutions to high energy



For small α we can see spurious discontinuous solutions

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DG: Simple Example

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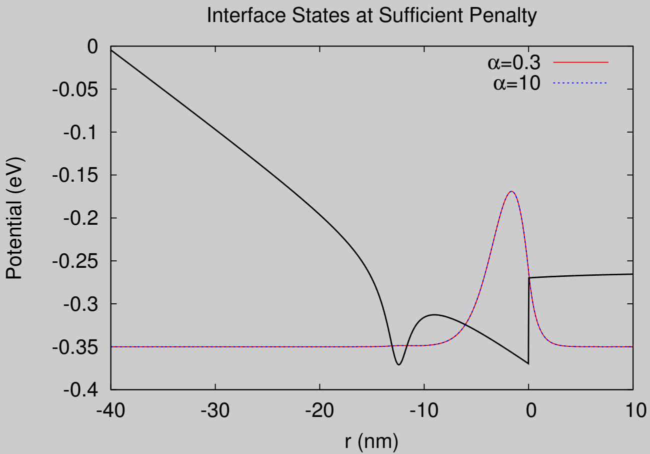
Parameter balances accuracy with conditioning



Large $\alpha \to$ small discontinuity, reduces diagonal dominance

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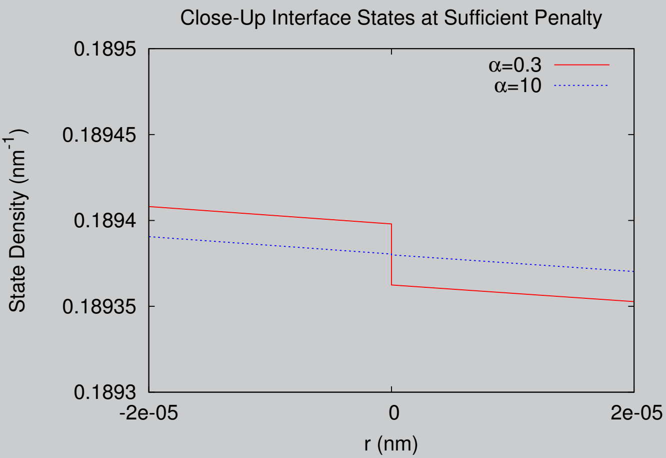
Discontinuity rigorously exists still



Controllable/negligible contribution to KE

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DG: Advantages and Plan

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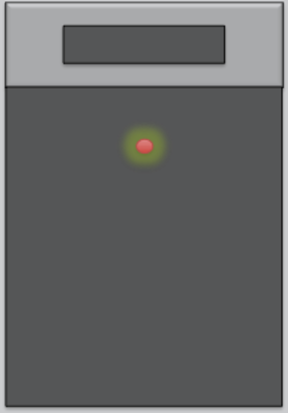
- Build a coarse mesh for electrostatics
- Forward QCAD solve w/o VO physics
- Extract quantum region $\rightarrow$ high order DG
- Local solvers adapt enriched basis



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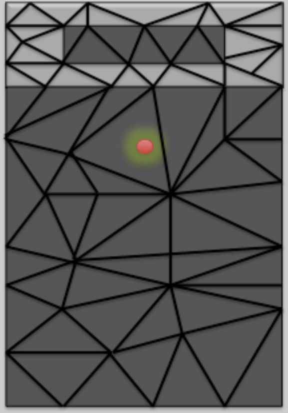

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DG: Advantages and Plan

- Construct CAD model of device
- Build a coarse mesh for electrostatics
- Forward QCAD solve w/o VO physics
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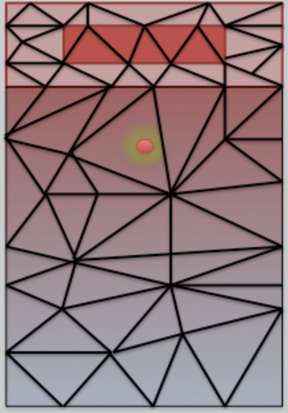

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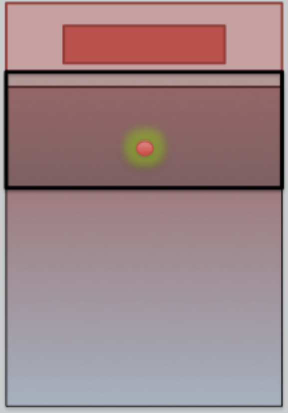

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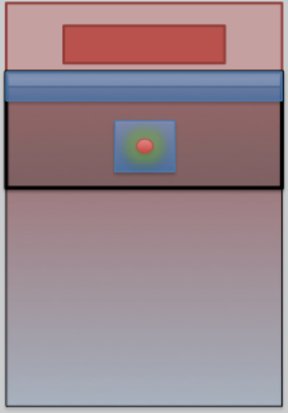

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Summary and Ongoing Work

Sandia National Laboratories

- **Summary:**
  - High fidelity numerical framework needed for complex models
  - Multi-valley EMT is numerically challenging
  - Discontinuous Galerkin methods are up to the challenge
- **Ongoing:**
  - Implementation of full 3D capability
  - Local adaptivity in space (and time)
  - Projective model reduction-based dynamics (stay for Toby's talk!)

Thank you for your attention!

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