Numerical Methods for the Design of 2-Well Quantum Devices

Chris Anderson

UCLA Mathematics Department

DARPA Quantum Information Science & Technology (QuIST) Program

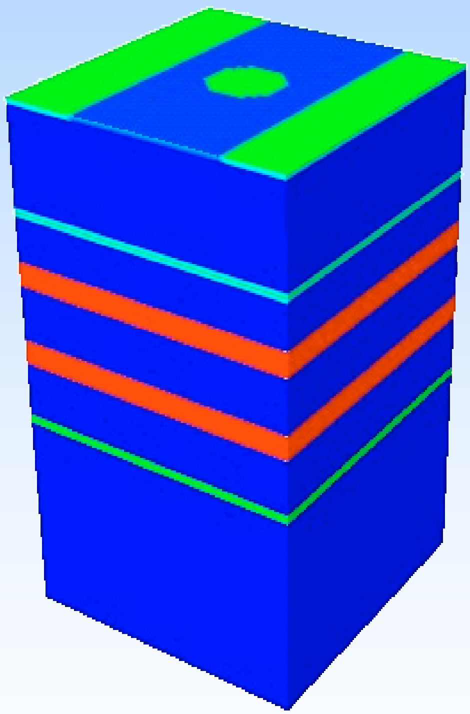
Collaborators :

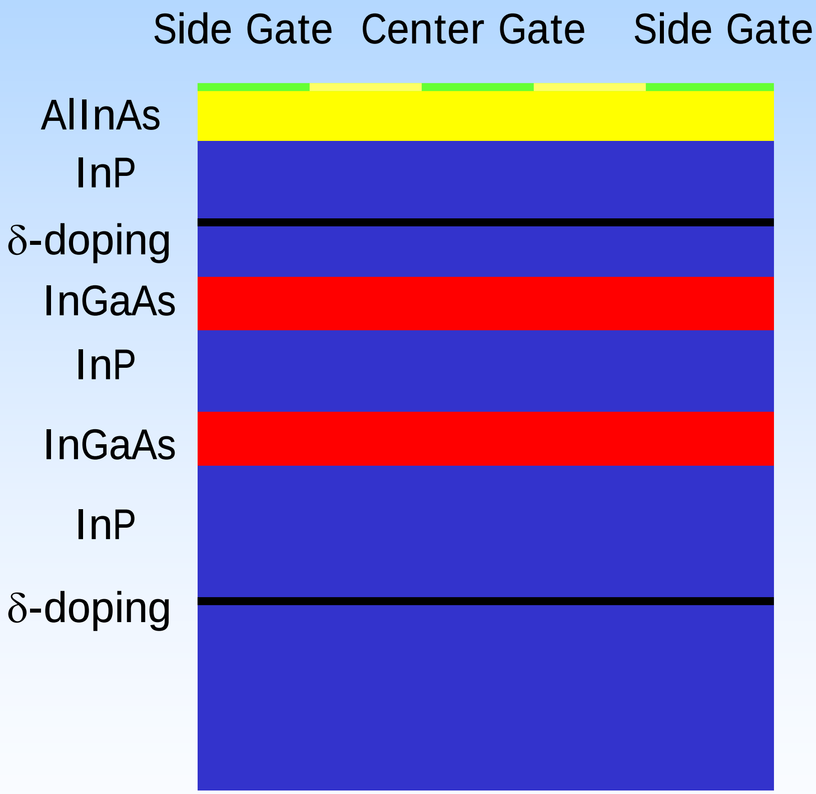
UCLA Math:	HRL Labs:	UCLA EE:
Russ Caflisch	Mark Gyure	Eli Yablanovitch
Derek Urwin	Geoff Simms	Hans Robinson
Tom Cecil	Ed Croke	

DEPARTMENT OF Mathematics AT UCLA

The Target Device:

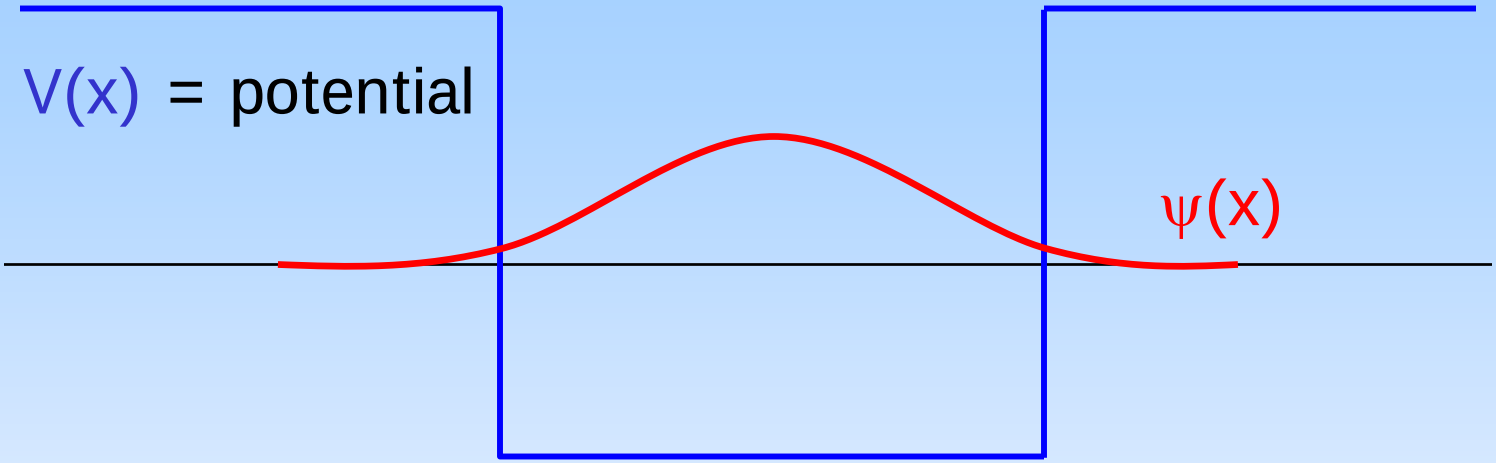
- Creates and confines a quantum dot electrostatically
- Senses dot using a quantum wire.





Device Structure

Single particle Schroedinger Equation



Single particle, 1 dimensional, time independent

Schroedinger's Equation

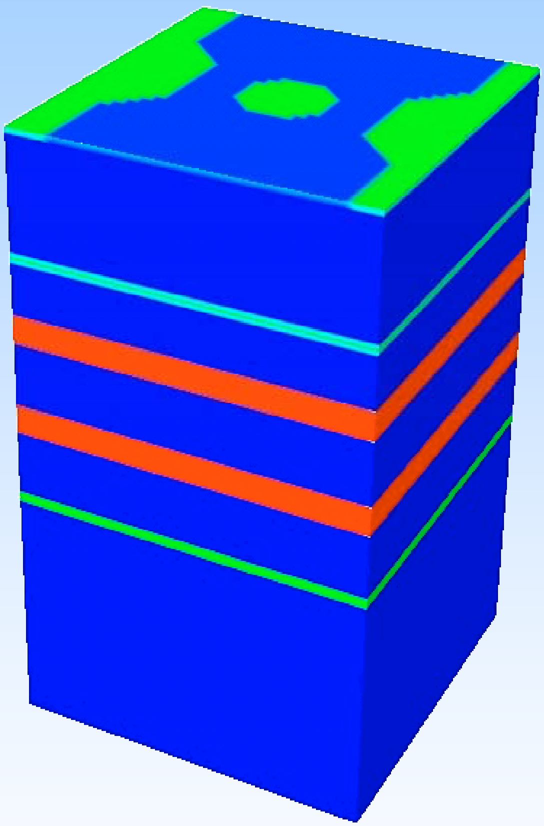
$$(-\hbar^2/2m)\frac{d^2\psi}{dx^2} + V(x)\,\psi = E\,\psi$$

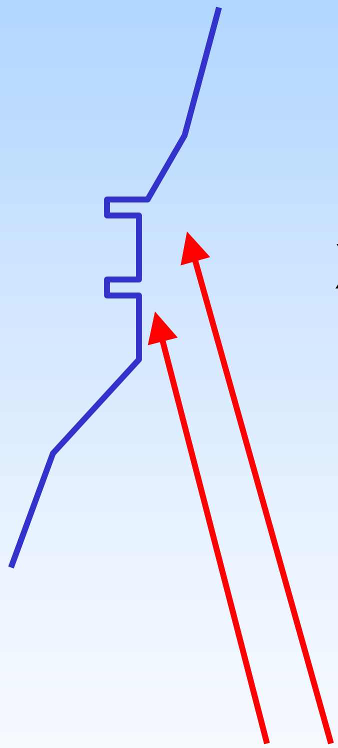
$\psi^* \psi$ = probability density for particle location

E = energy of the particle

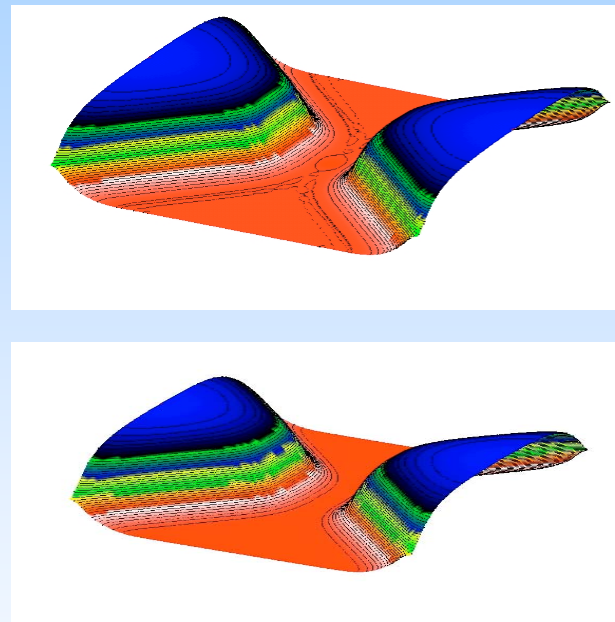
3D

V(x,y,z) =





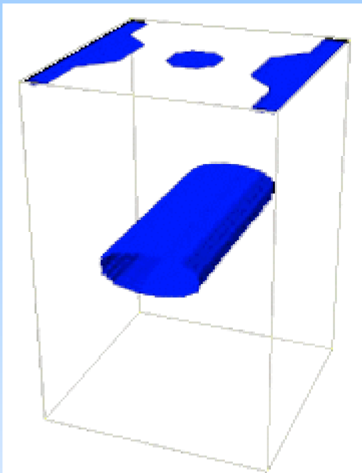
X



Trap electrons: vertically in quantum “wells”

transversely using gate potentials

Device Operation:

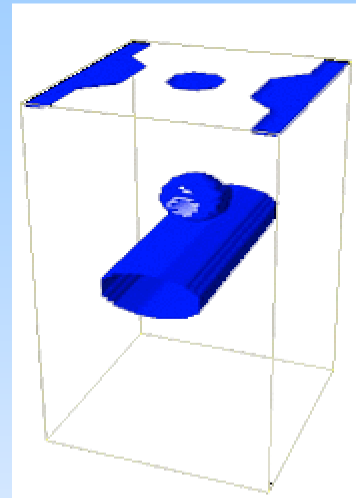


Side voltage applied

⇩

quantum wire

Multiple states in the lower well.
Confinement in 2 directions.



Side and dot voltage applied

⇩

quantum wire + quantum dot

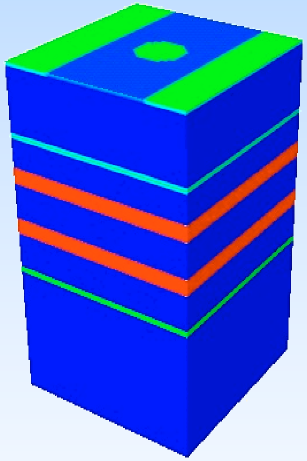
Single state in the upper well.
Confinement in 3 directions

Multiple states in the lower well.
Confinement in 2 directions

Goal of the computational simulations:

To help those involved in building the device make intelligent design decisions.

Design decisions?



How thick should the wells be?

How wide should the center dot gate be?

Should the side gates be wedges or strips?

How much δ doping should there be?

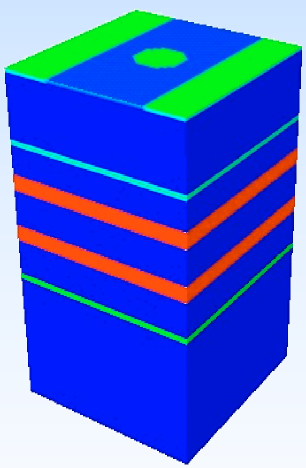
What is the impact of variations in the δ doping?

*
*
*

Modeling

Simplest model that provides useful answers.

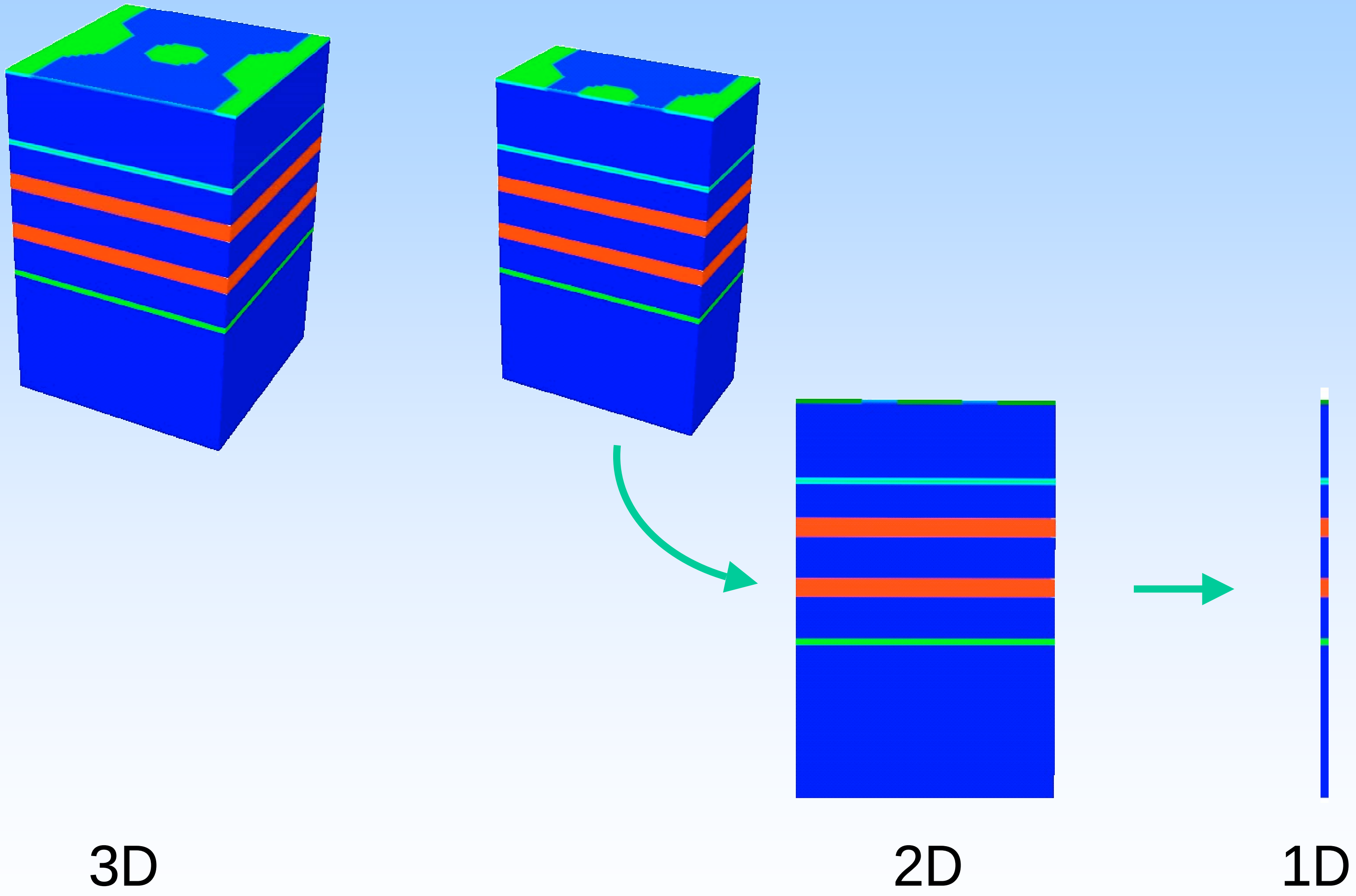
Complete Physics



Perturbations of SP ← Gyure

Anderson
Caflisch → Schroedinger Poisson (SP)

Use Dimension reduction



Equations

Coupled Poisson-Schroedinger equations

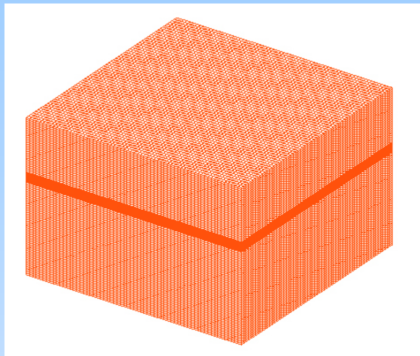
$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma \, \delta_{sources} + \Sigma \, G(\lambda_k, \psi_k)$ ϕ : potential

$- \nabla \cdot ((\hbar^2 / 2m) \nabla \psi) + (\phi + U) \psi = \lambda \psi$ ψ : wave functions

Computational tasks:

- (I) Eigenvalue/Eigenvector problem
- (II) Solution of Poisson's equation
- (III) Self consistent solution

Discrete Equations



$\vec{\phi}$, $\vec{\psi}$: vectors of values at nodes of grid $\in R^{n_x n_y n_z}$

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k, \psi_k)$$

$$\Longrightarrow \quad L \vec{\phi} = \vec{P} + \vec{f}(\vec{\psi})$$

$$- \nabla \cdot ((\hbar^2 / 2m) \nabla \psi) + (\phi + U) \psi = \lambda \psi$$

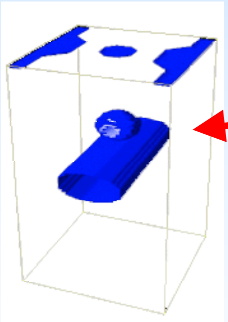
$$\Longrightarrow \quad S \vec{\psi} + \vec{V}(\vec{\phi}) = \lambda \vec{\psi}$$

(I) Eigenvalue/Eigenvector problem

$$- \nabla \cdot ((\hbar^2 / 2m) \nabla \psi) + (\phi + U) \psi = \lambda \psi$$

Challenges:

- 3D ($\vec{\psi} \in R^{n_x n_y n_z}$)
- A large number of eigenvectors/eigenvalues must be computed



Many wave functions comprise the quantum wire

- Eigensystem must be re-computed for each self-consistent iteration.

(I) Eigenvalue/Eigenvector problem

$$- \nabla \cdot ((\hbar^2 / 2m) \nabla \psi) + (\phi + U) \psi = \lambda \psi$$

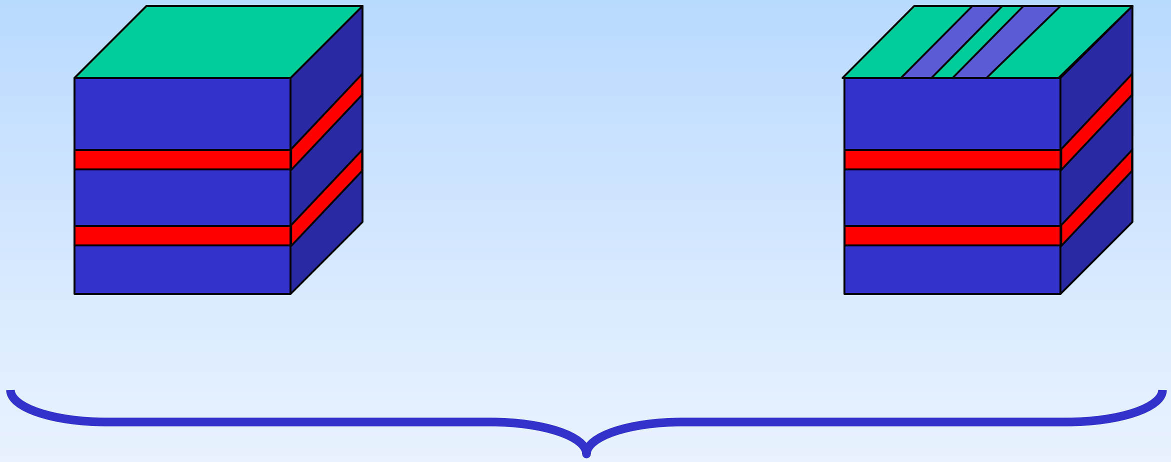
The eigenvalues/eigenvectors can be obtained with standard methods...

but you will have to wait awhile (days).

How have results been obtained more rapidly?

(I) Approach

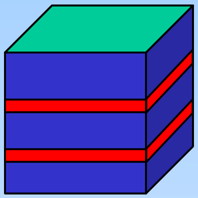
Change the problem so that the eigenproblem can be solved more efficiently.



Take advantage of special geometry : 1D and 2D Shroedinger-Poisson equation idea.

1D and 2D Schroedinger-Poisson

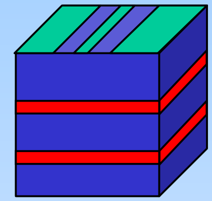
1D-SP



$\phi(x,y,z) = \alpha(z)$

$\psi(x,y,z) = \gamma(z)\, e^{ikx}\, e^{iky}$

2D-SP



$\phi(x,y,z) = \alpha(z,x)$

$\psi(x,y,z) = \gamma(z,x)\, e^{ikx}$

← Separate variables - be clever (density of states technique) →

$$\frac{d}{dz}\left(\varepsilon\ \frac{d\alpha}{dz}\right) = \sum \delta_s + \sum_k \mathrm{G}_{1D}(\gamma_k, \lambda_k)$$

$$\frac{d}{dz}\left(\frac{\hbar^2}{2m}\ \frac{d\gamma}{dz}\right) + (\alpha + U)\ \gamma = \lambda\ \gamma$$

1D Poisson

1D Schroedinger

$$\nabla(\varepsilon\ \nabla\alpha) = \sum \delta_s + \sum_k \mathrm{G}_{2D}(\gamma_k, \lambda_k)$$

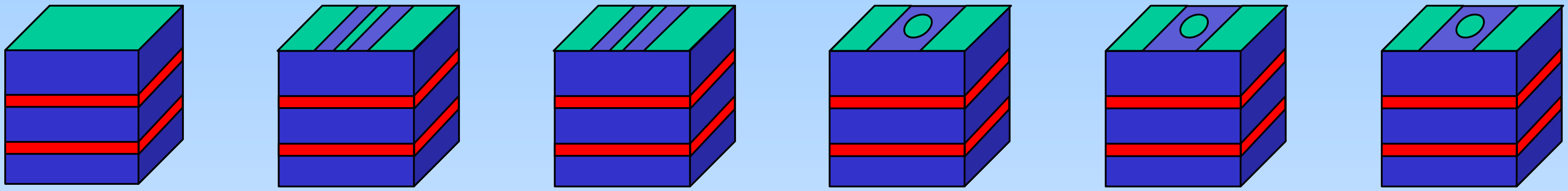
$$\nabla\left(\frac{\hbar^2}{2m}\ \nabla\gamma\right) + (\alpha + U)\ \gamma = \lambda\ \gamma$$

2D Poisson

2D Schroedinger

Family of approximations:

1D-SP | 2D-SP | SP



$\phi = \alpha(z)$

$\psi = \gamma(z)\, e^{ikx}\, e^{iky}$

$\phi = \alpha(z, x)$

$\psi = \gamma(z, x)\, e^{iky}$

$\phi(x,y,z) \approx \alpha(z) + \beta(x)$

$\psi(x,y,z) = \gamma(z)\, \mu(x)\, e^{iky}$

2D Poisson

2 x 1D Schroedinger

$\phi(x,y,z) \approx \alpha(z) + \beta(x) + \chi(y)$

$\psi(x,y,z) = \gamma(z)\, \mu(x)\, \varpi(y)$

3D Poisson

3 x 1D Schroedinger

$\phi(x,y,z) \approx \alpha(z) + \beta(x,y)$

$\psi(x,y,z) = \gamma(z)\, \mu(x,y)$

3D Poisson

1D Schroedinger +
2D Schroedinger

The Equations We Actually Solve

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k, \psi_k)$$

$$- \nabla \cdot \left((\hbar^2 / 2m) \nabla \psi \right) + (\tilde{\phi} + U)\, \psi = \lambda\, \psi$$

$\tilde{\phi} = \alpha(z)$	1D Poisson	1D Schroedinger
$\tilde{\phi} = \alpha(z) + \beta(x)$	2D Poisson	2 x 1D Schroedinger
$\tilde{\phi} = \alpha(z) + \beta(x,y)$	3D Poisson	1D Schroedinger + 2D Schroedinger

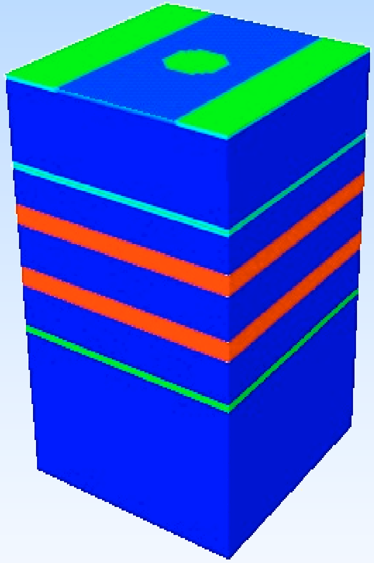
CPU work required for 1D & 2D operators << 3D operator

(II) Poisson Equation

$$\nabla \cdot (\varepsilon \nabla \phi) = f(x,y,z)$$

Issues:

- 3D $(\vec{\phi} \in R^{n_x n_y n_z})$
- Discontinuous coefficients
- Thin layers
- Non-trivial geometry



Poisson Equation

$$\nabla \cdot (\varepsilon \nabla \phi) = f(x,y,z)$$

The solution can be obtained with standard methods...

but they don't take advantage of the special features of the problem.

(II) Solution Technique:

Use “analytic” x 2D Fourier basis:

$$\phi(z,x,y) = \sum_{k_1,k_2} a_{k_1,k_2}(z)\ \mathrm{e}^{ik_1\frac{x}{dX}}\ \mathrm{e}^{ik_2\frac{y}{dY}}$$

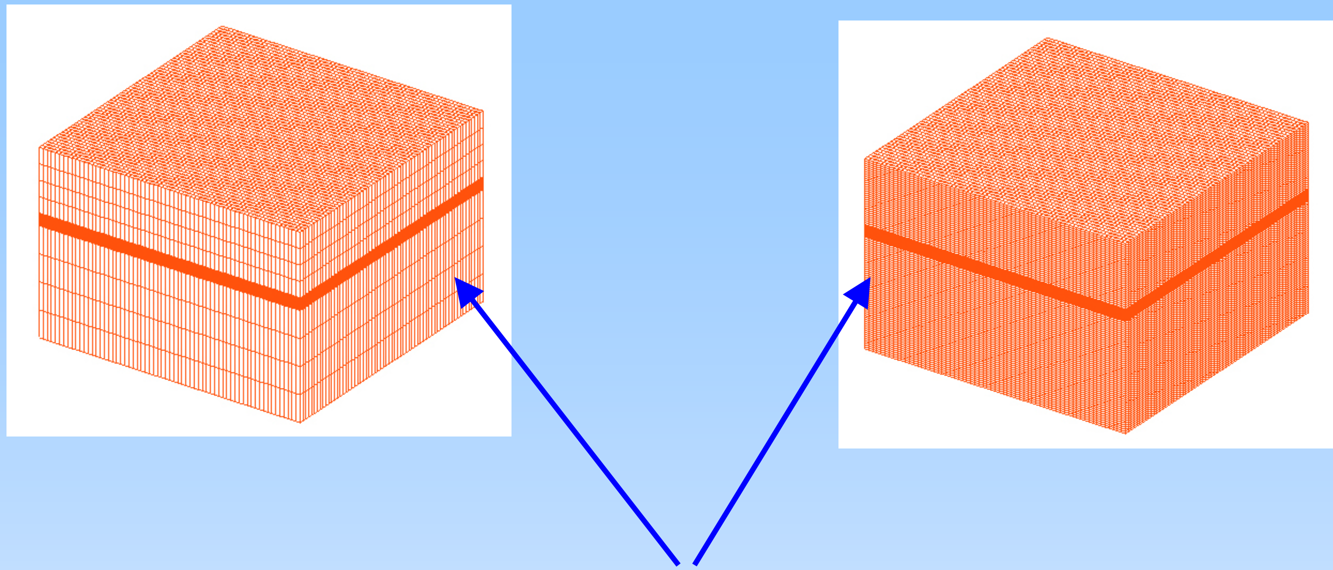
2D Fourier transform at each z $\Rightarrow$

$$\frac{d}{dz}(\varepsilon\ \frac{da_{k_1,k_2}(z)}{dz}) - \left(\frac{4\pi k_1^2}{dX^2} + \frac{4\pi k_2^2}{dY^2}\right) a_{k_1,k_2}(z) = \hat{f}_{k_1,k_2}(z)$$

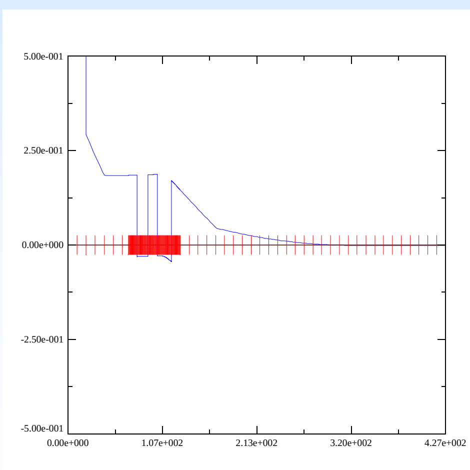
Use piecewise analytic solution of 1D equation (extension of Wachspress’s idea) and analytic inclusion of δ function sources.

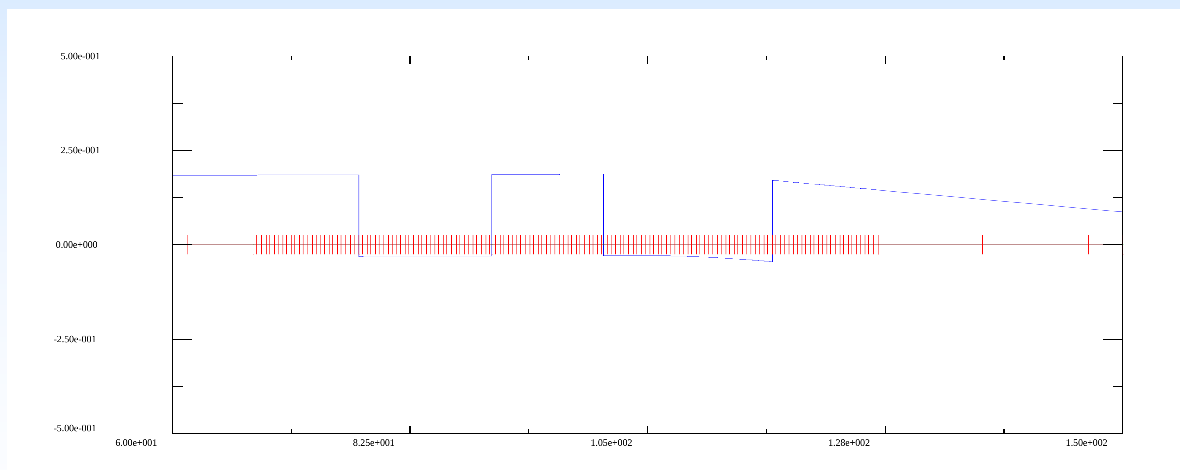
(II) Features:

- Exact in harmonic regions
- Allows extreme refinement in z-direction
- High accuracy
- Non-iterative & “Fast” ≈ $O(n_z n_x n_y \log(n_x n_y))$

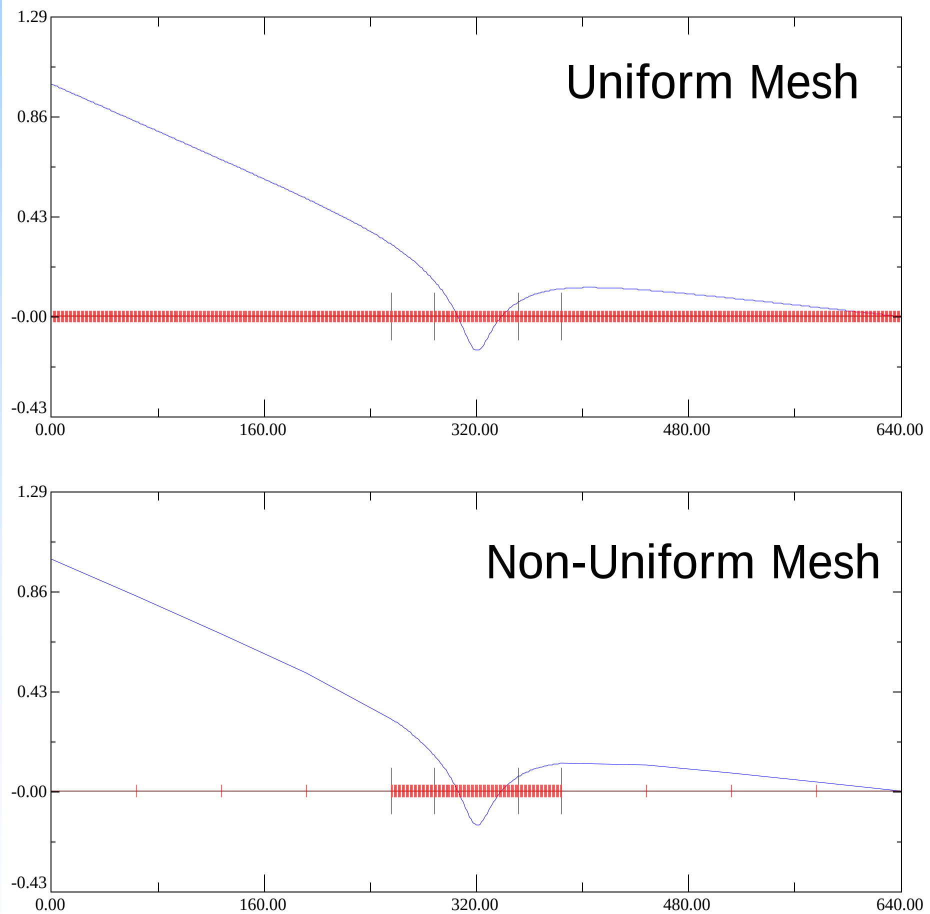


Equivalent accuracy near wells, even with "extreme" coarsening in the vertical direction.





(II) Accuracy with extreme mesh coarsening:



ϕ along center line (z-axis)

Max. Error

Finite volume	Analytic X Fourier (2)	Analytic X Fourier (4)
8.44-04	2.07-04	1.96-06
6.80e-03	2.07-04	1.96-06

Accuracy unchanged --- and requires only 1/10 CPU time!

(III) Self-Consistency

Schrodinger-Poisson

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k, \psi_k)$$

$$- \nabla \cdot ((\hbar^2 / 2m) \nabla \psi) + (\phi + U) \psi = \lambda \psi$$

Transform
to Non-linear Poisson

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k (\phi), \psi_k(\phi))$$

$$L(\phi) \quad = \quad S \quad + \quad F(\phi)$$

(III) Self-Consistency

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k(\phi), \psi_k(\phi))$$

$$\downarrow \qquad \downarrow \qquad \downarrow$$

$$L(\phi) = S + F(\phi)$$

Discrete?

$$L(\vec{\phi}) = \vec{S} + \vec{F}(\vec{\phi})$$

$n_z n_x n_y$ non-linear equations in $n_z n_x n_y$ unknowns

Self consistent iteration story ...

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma\, \delta_{sources} + \Sigma\, G(\lambda_k(\phi), \psi_k(\phi))$$

Gradient methods: Newton & quasi-Newton

$\Rightarrow$ requires gradients of $\Sigma\, G(\lambda_k(\phi), \psi_k(\phi))$

Derivatives of G are not continuous in zero temperature limit.

Evaluation of the derivatives is complicated.

Robust convergence behavior requires careful iteration design.

Highly dimension dependent code.

Return to "simple" iteration

$$\nabla \cdot (\varepsilon \nabla \phi^{n+1}) = \Sigma \delta_{sources} + \Sigma G(\lambda_k(\phi^n), \psi_k(\phi^n))$$

$$(L(\phi^{n+1}) = S + F(\phi^n))$$

Easy to implement.

Iteration procedure is dimension "independent"

Iteration doesn't always converge.

Introduce a relaxation parameter:

$$L(\phi^*) = S + F(\phi^n)$$

$$\phi^{n+1} = (1-\alpha)\phi^n + \alpha \phi^*$$

“simple” iteration with relaxation

$L(\phi^*) = S + F(\phi^n)$

$\phi^{n+1} = (1-\alpha)\phi^n + \alpha\, \phi^*$

Requires small α to get convergence $\Rightarrow$ 100’s of iterations

Fix?

We observe that “simple” iteration is just Euler’s method with timestep α applied to

$$\frac{\partial \phi}{\partial t} = L^{-1}(S + F(\phi)) - \phi$$

Equivalence to Eulers's method

$L(\phi^*) = S + F(\phi^n)$

$\phi^{n+1} = (1-\alpha)\phi^n + \alpha\,\phi^*$

$\Rightarrow \quad \phi^{n+1} = \phi^n + \alpha\,(L^{-1}(S + F(\phi^n)) - \phi^n)$

$\Rightarrow \quad \dfrac{(\phi^{n+1} - \phi^n)}{\alpha} = L^{-1}(S + F(\phi^n)) - \phi^n$

$\Rightarrow$ Euler's method with timestep α applied to

$$\frac{\partial\phi}{\partial t} = L^{-1}(S + F(\phi)) - \phi$$

Using This Observation

The need for small α for convergence $\Longrightarrow$ "stiff" ODE.

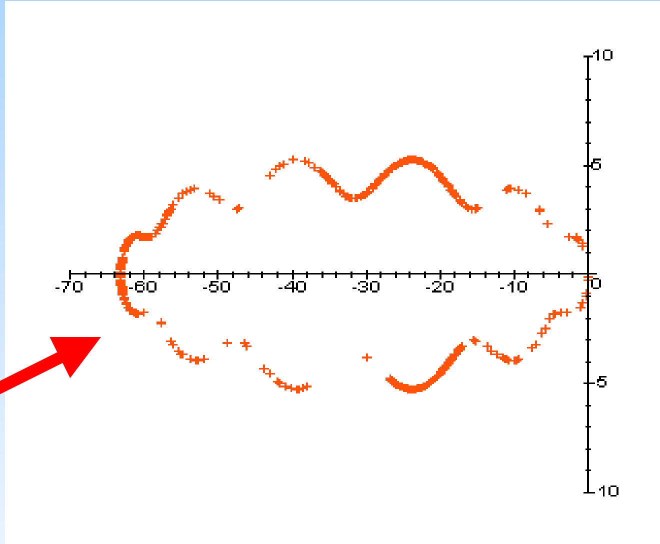
Euler's method is not a good way to solve "stiff" ODE's.

So use an alternate ODE method …

Stabilized Runge-Kutta Methods

$$
\begin{aligned}
k_1 &= dt * f(y_m) \\
k_2 &= dt * f(y_m + \alpha_1^1\ k_1) \\
k_3 &= dt * f(y_m + \alpha_1^2\ k_1 + \alpha_2^2\ k_2) \\
&\ \vdots \\
k_n &= dt * f(y_m + \alpha_1^{n-1}\ k_1 + \alpha_2^{n-1}\ k_2 + + \cdots + \alpha_{n-1}^{n-1}\ k_{n-1}) \\
y_{m+1} &= y_m + \alpha_1^n\ k_1 + \alpha_2^n\ k_2 + \cdots + \alpha_n^n\ k_n
\end{aligned}
$$

For steady state calculations -- use first order methods with extra stages chosen to possess large regions of absolute stability.



n stages $\Longrightarrow$ There is a method whose region of absolute stability contains $[-\gamma\, n^2, 0]$ for $0 < \gamma < 2$.

(III) Solution Technique

$$\nabla \cdot (\varepsilon \nabla \phi) = \Sigma \delta_{sources} + \Sigma G(\lambda_k(\phi), \psi_k(\phi))$$

$$\downarrow \qquad \downarrow \qquad \downarrow$$

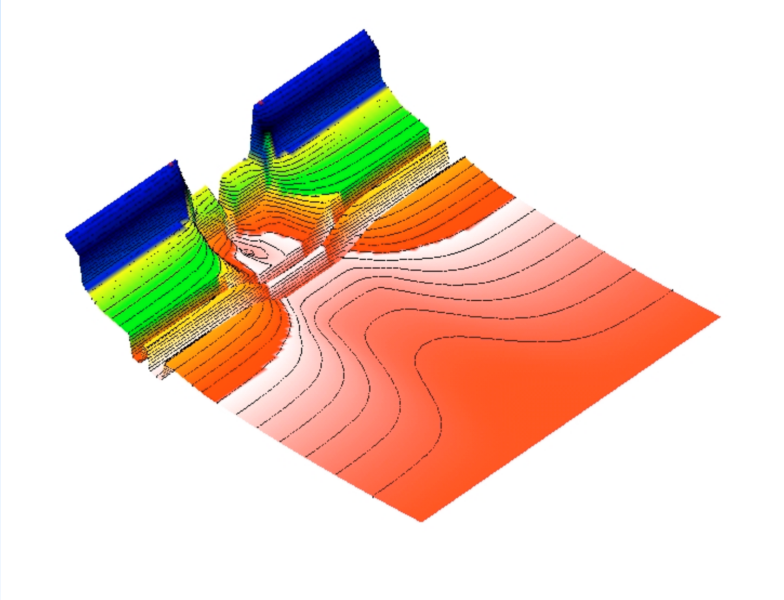
$$L(\phi) = S + F(\phi)$$

"Evolve" to the solution by solving

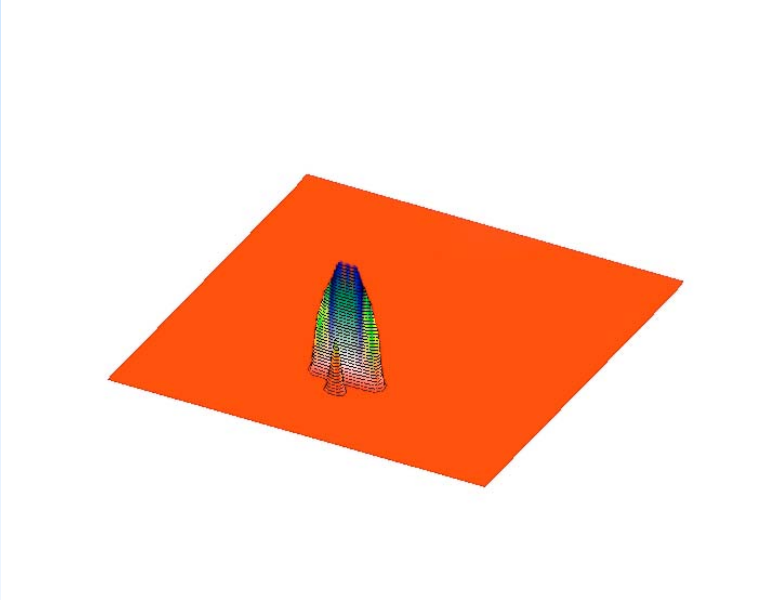
$$\frac{\partial \phi}{\partial t} = L^{-1}(S + F(\phi)) - \phi$$

to steady state using a custom Runge-Kutta ODE method.

Sample 2D Results

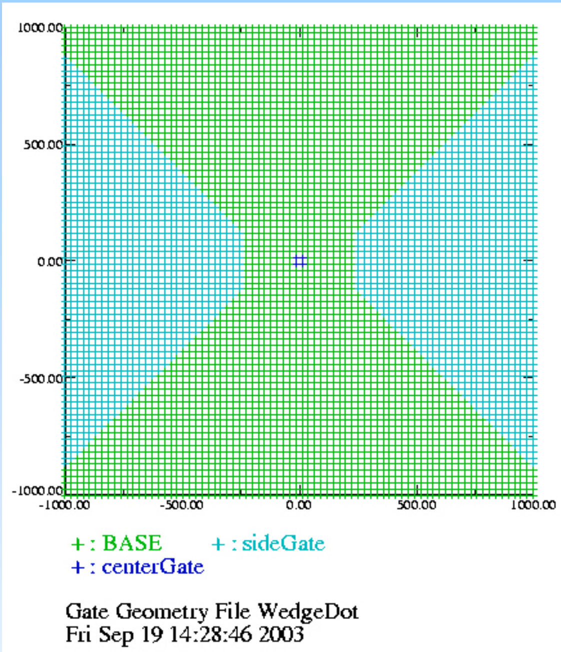


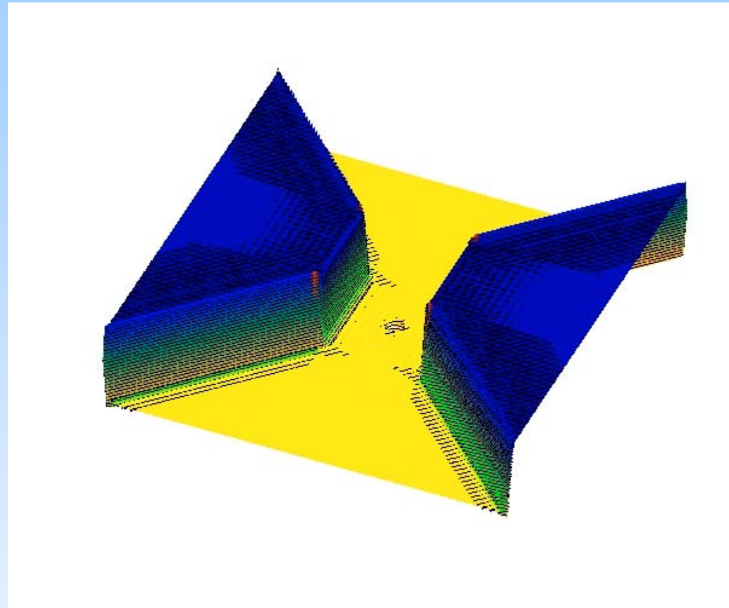
Potential + band offset



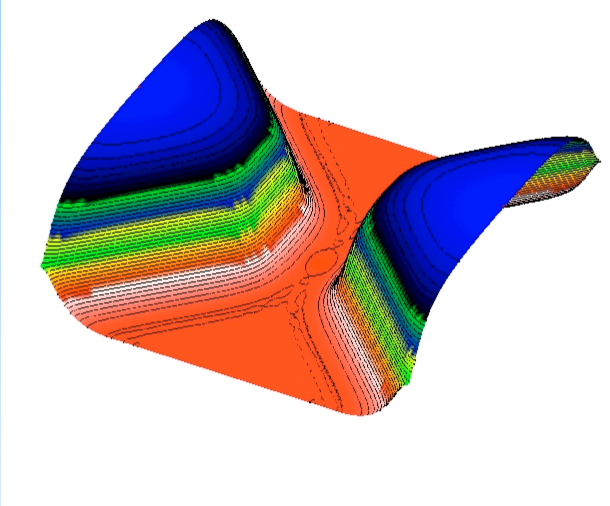
Charge density

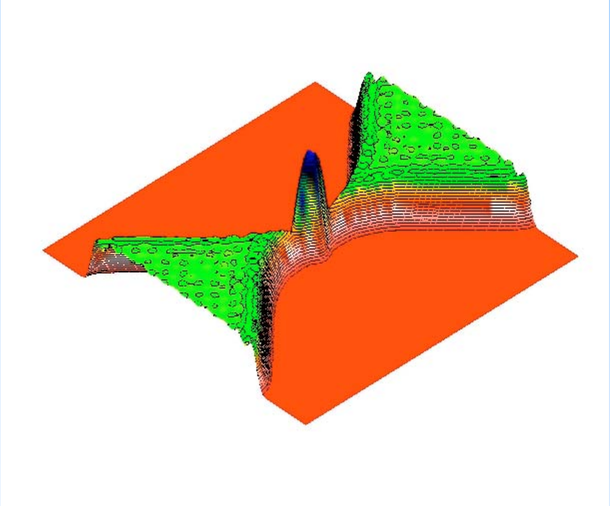
3D Results

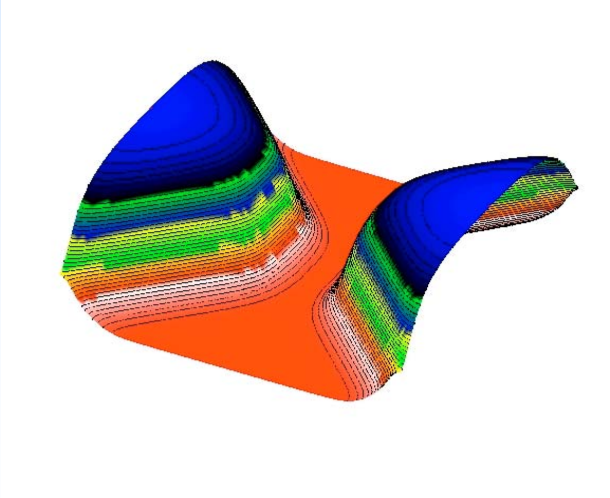

1000.00
500.00
0.00
-500.00
-1000.00
-1000.00
-500.00
0.00
500.00
1000.00
+ : BASE
+ : sideGate
+ : centerGate
Gate Geometry File WedgeDot
Fri Sep 19 14:28:46 2003

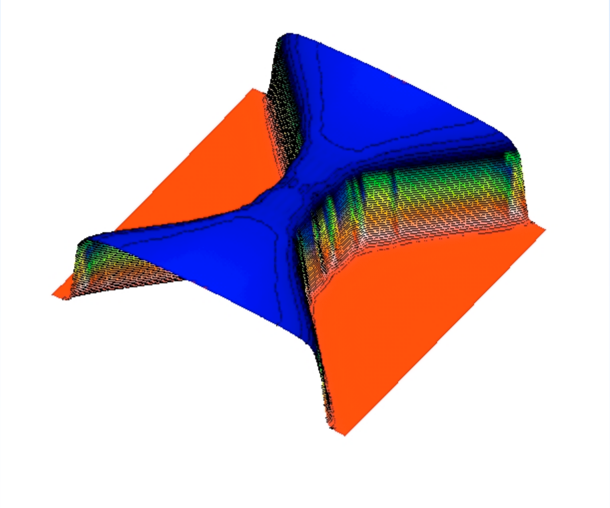


3D Results









Why the need for speed?

We want to explore parameter space …

Parametric database construction and evaluation