Extreme Scale EDA: From Molecules to Vehicles

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with Using slides borrowed from

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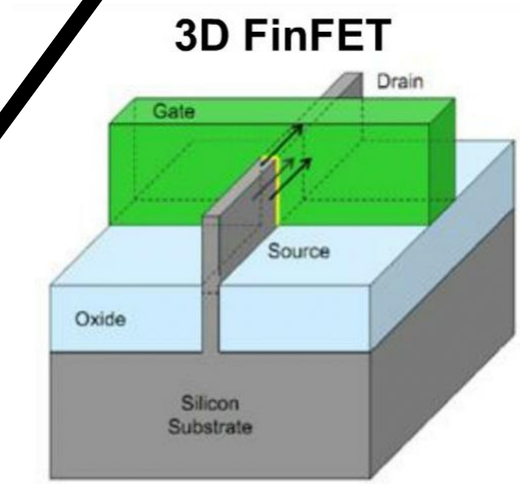
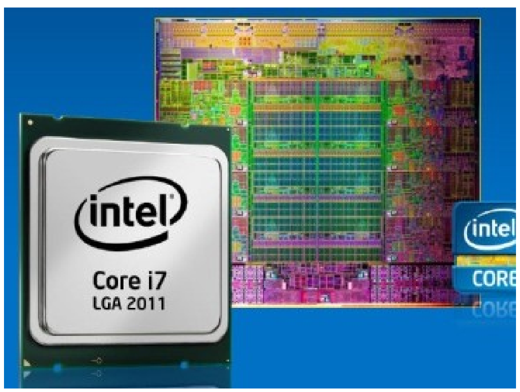
What’s Harder

← 3 Meters →

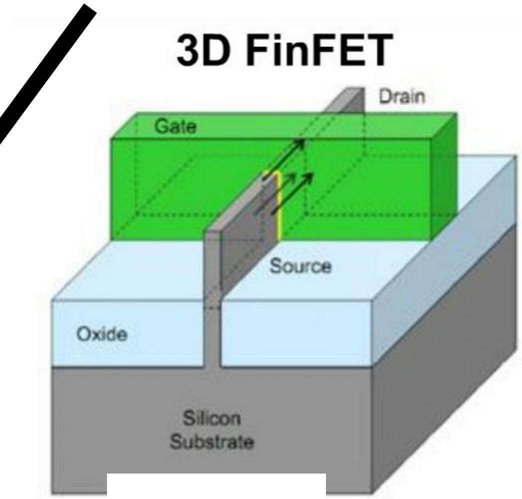


$=10^9$

← 3 NM →



←→

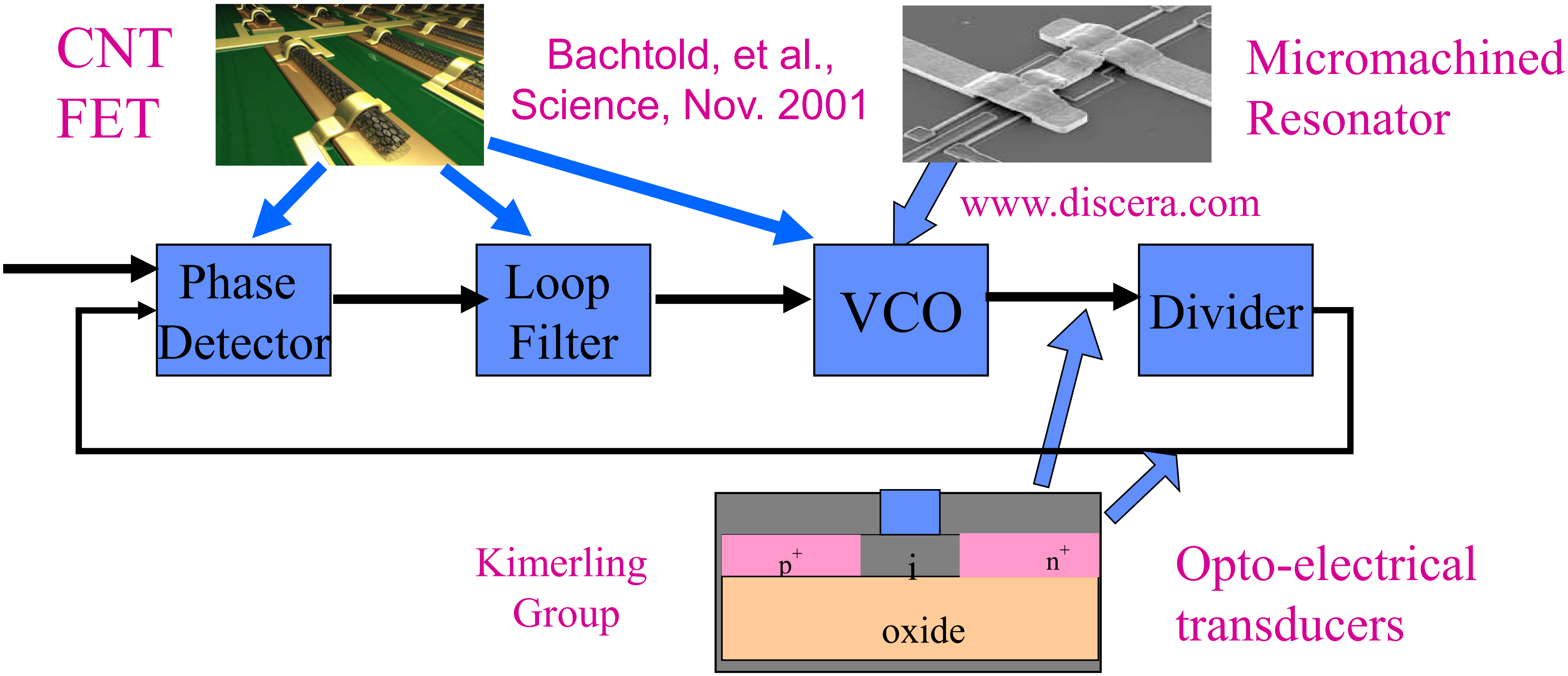


$=10^7$

← 3 NM →

Cars are 100x harder to design than CPUs.

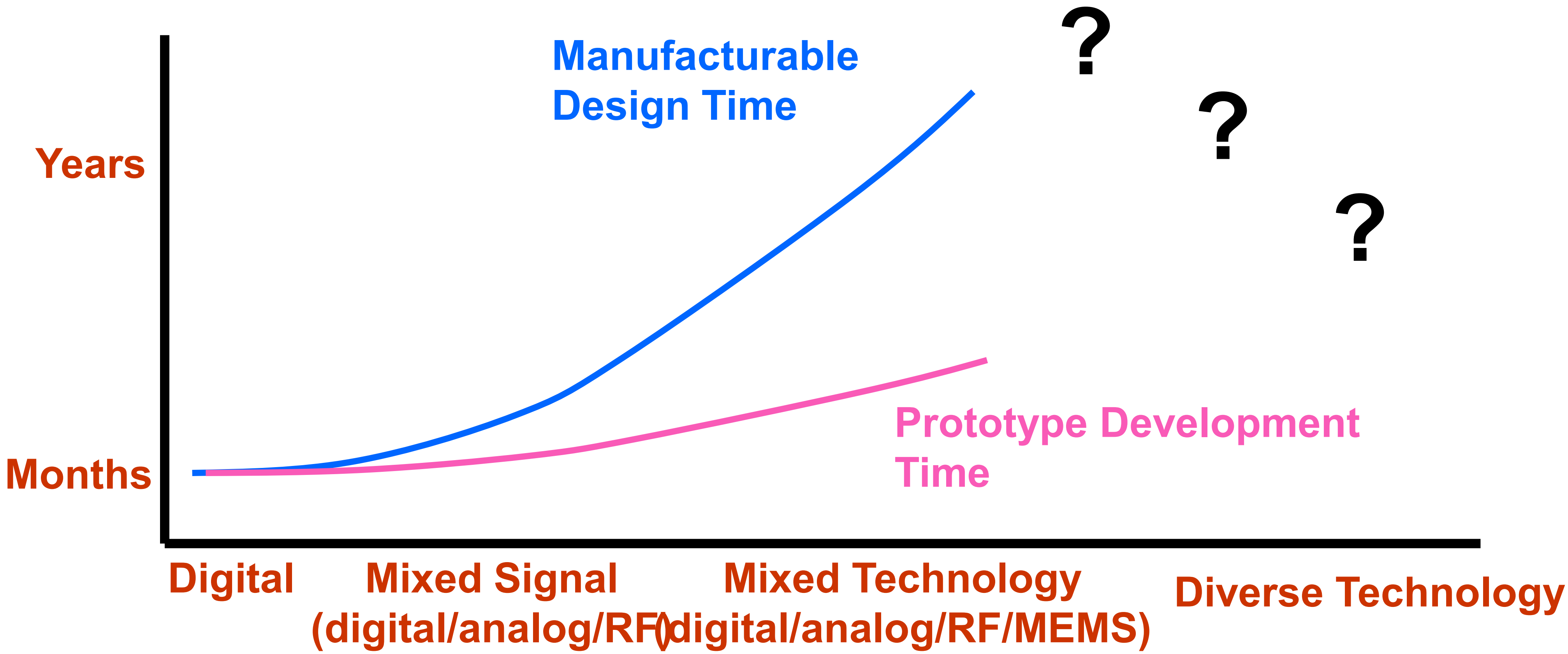
A Multitechnology Phase-Locked Loop



Evaluating the New Technology

- What is system performance (capture, lock, noise, etc)?
- What is the impact of modifying technology parameters?
- How tight must manufacturing tolerances be?

Manufacturable Design Time Exploding with Technology Diversity



- **Better Computational Tools Are the Only Solution**
  - Physical Prototyping Leads to One-of Designs
  - Models needed to understand impact of process variations
  - Optimization Needed to find More Manufacturable Designs

Enabling Conceptual Design of Manufacturable Diverse Technology

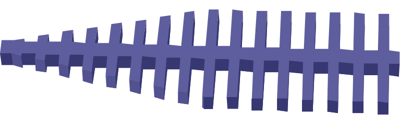
Parameterized Model Reduction, Dimension Reduction (3-D →2D)

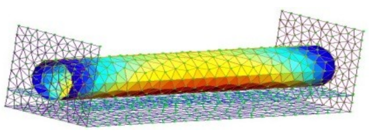
Parameterized Models

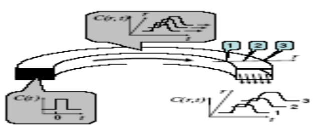
$$\frac{dx_r(t)}{dt} = \qquad +$$

$$y(t) =$$

Robust Optimization (Primal-Dual Interior Point Methods)







Physical Models

Fast Solvers (Multiresolution, PFFT)

Implicit Hession Approaches

$$min_x max_{p\in\Omega} f(x,p)$$

$$g(x,p) = 0, \forall p \in \Omega$$

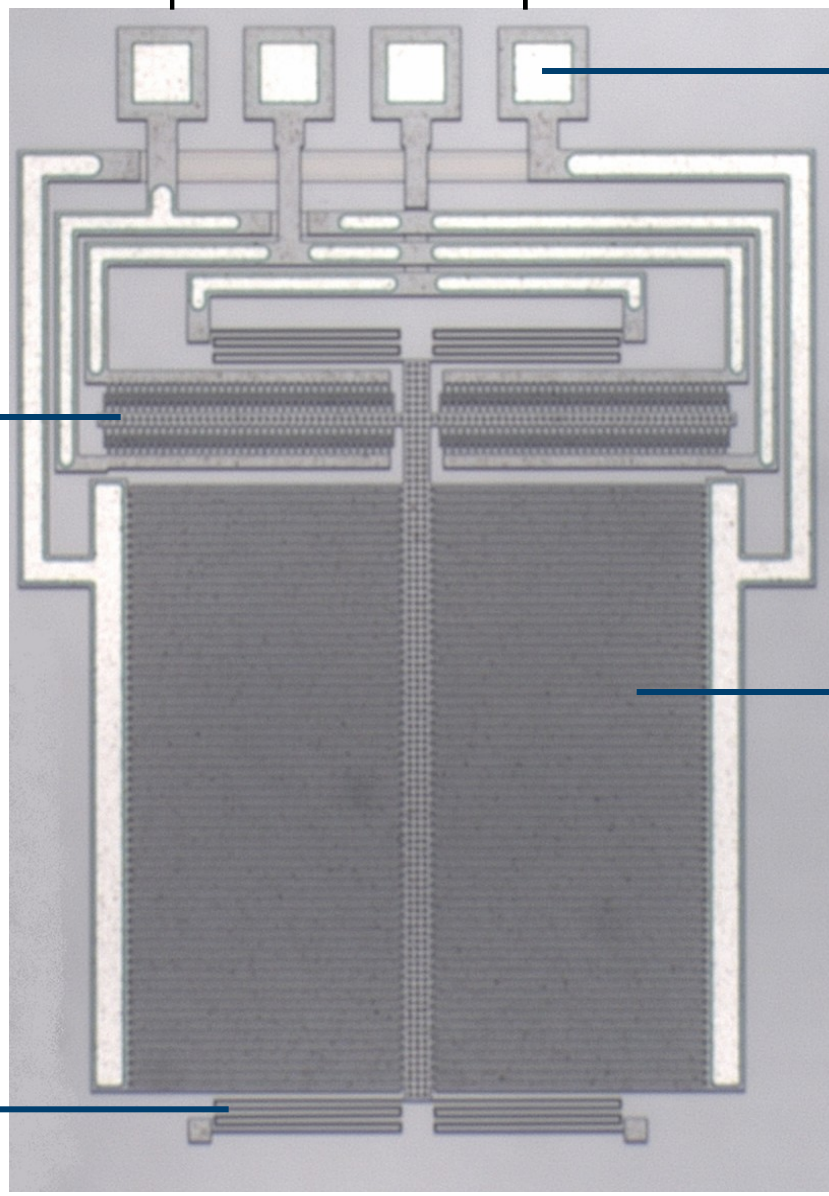
$$h(x,p) \leq 0, \forall p \in \Omega$$

- **Combine Robust Optimization with Physical Simulation**
- **Generic approaches to address Diverse Technology**
- **Extract parameterized models to address complex systems**

Casimir Experiments (Slide thanks to R. Ardito)

Layout: overall dimensions 1000x1500μm

optical microscope view



Driving comb finger capacitors

2x37 elements
gap 1.6μm
initial overlap 14μm

Actuation pads

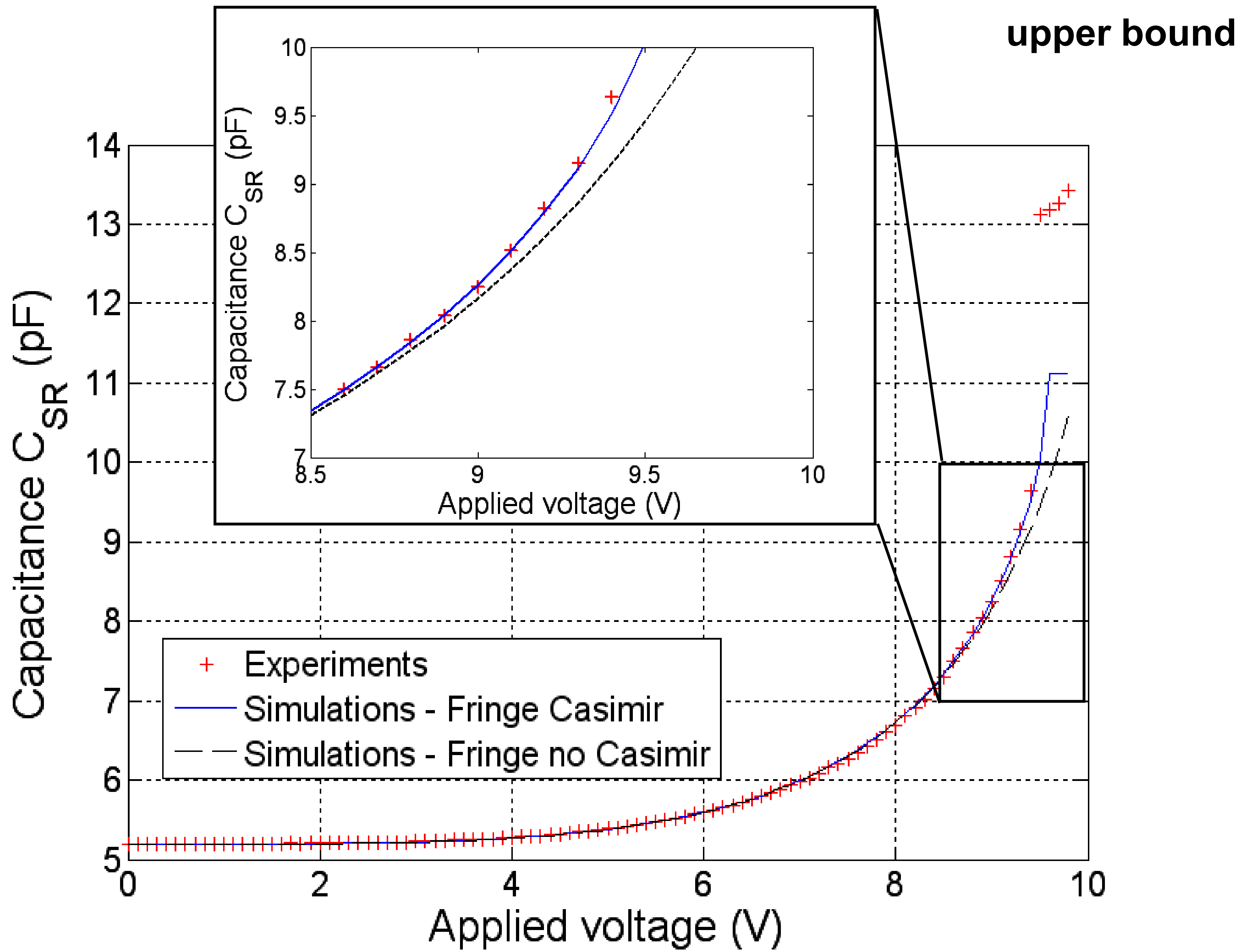
Folded springs

5-folded
width 2μm
length 250μm

Sensing parallel plate capacitors

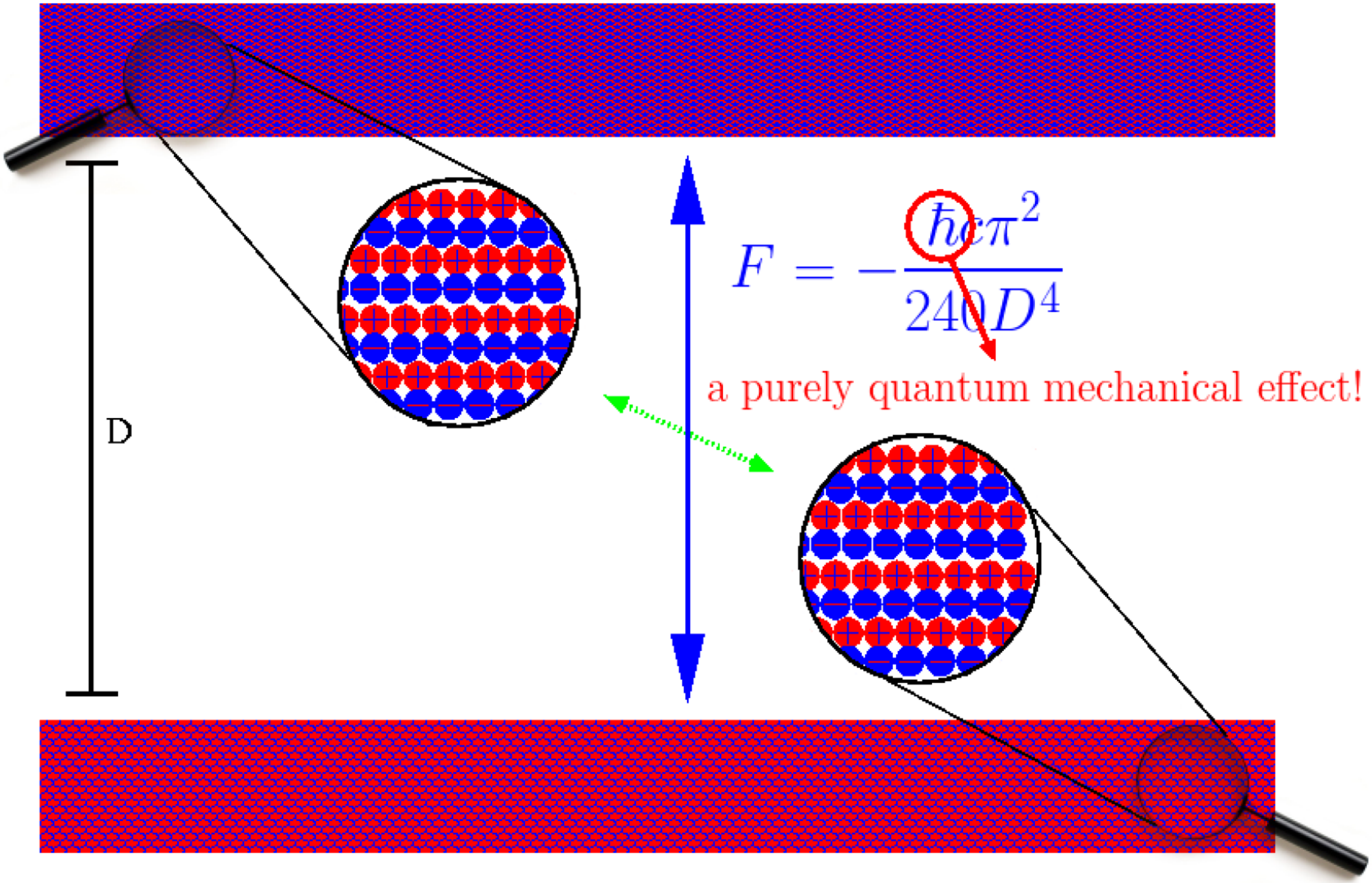
2x60 elements
initial gap 1.6μm
length 360μm

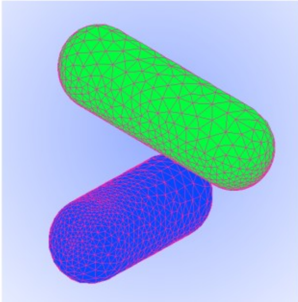
Capacitance versus voltage suggests Casimir force



What Are Casimir Forces?

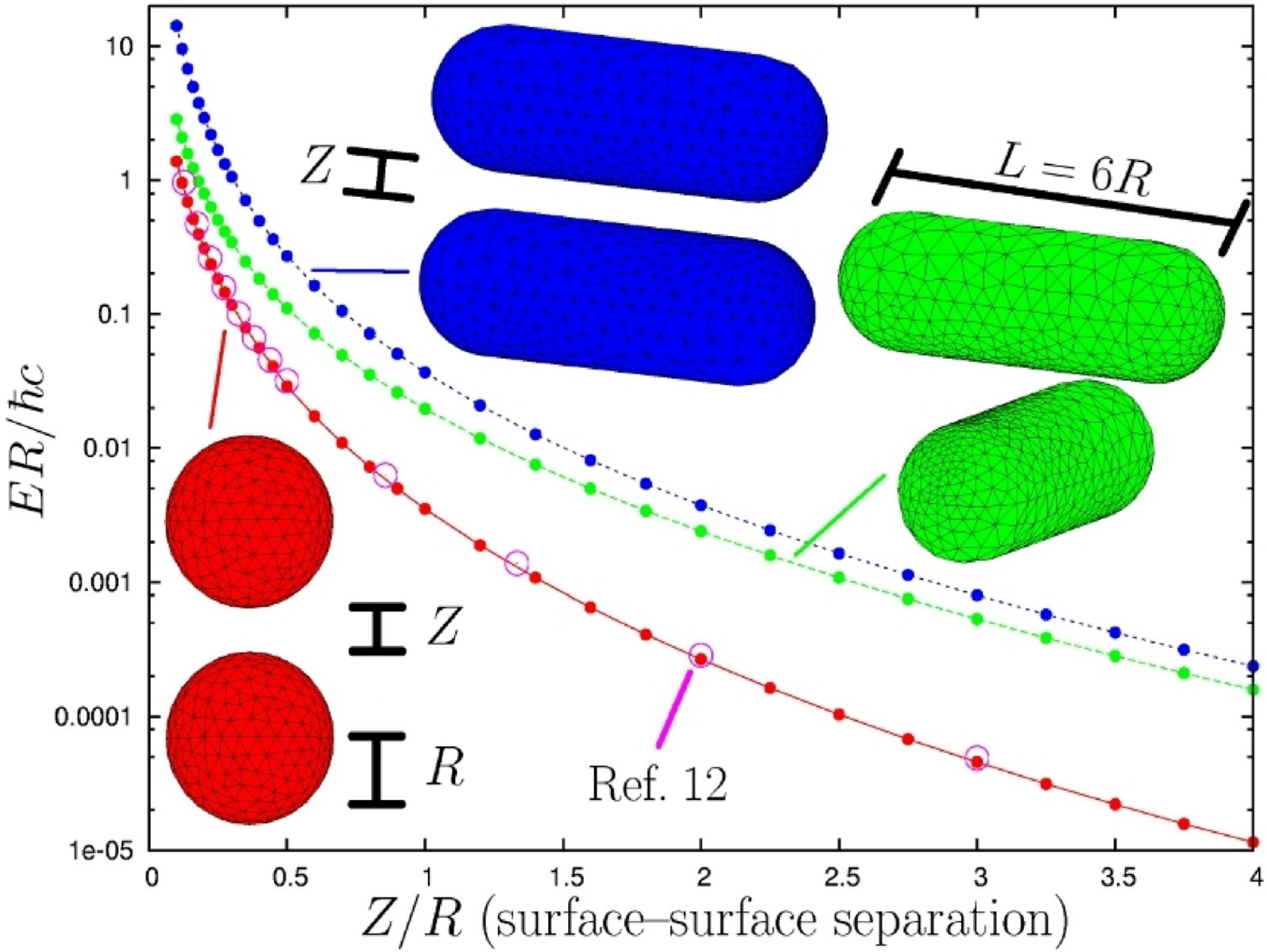
The Casimir effect is a *purely quantum phenomenon* and thus is *not captured by any existing NEMS modeling software.*





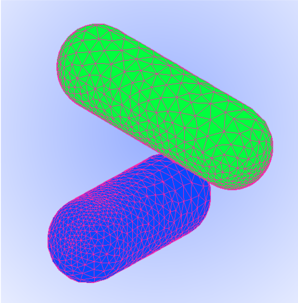
Results: Spheres, Parallel & Crossed Capsules

Validation of 3D code

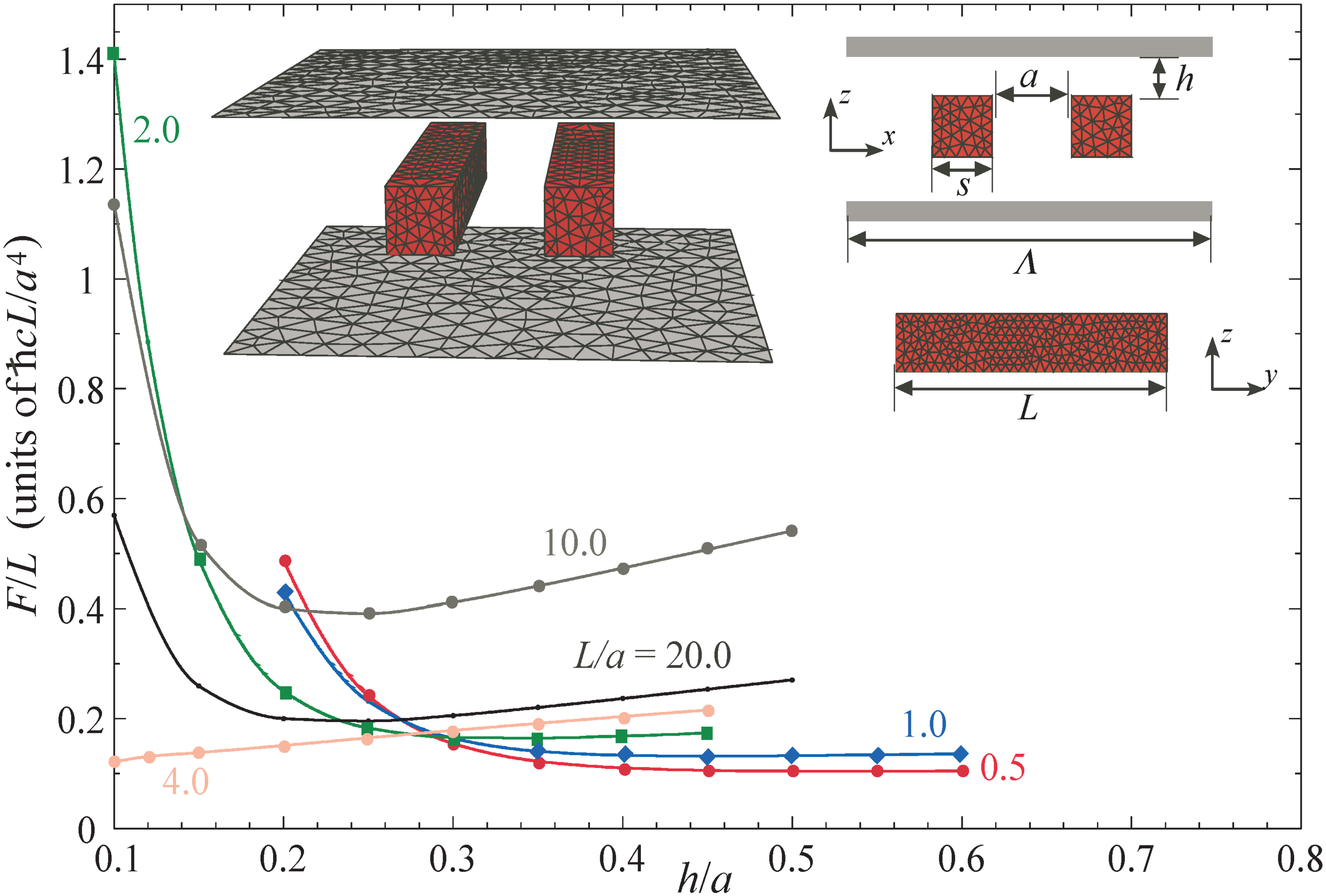


Computing Casimir Forces

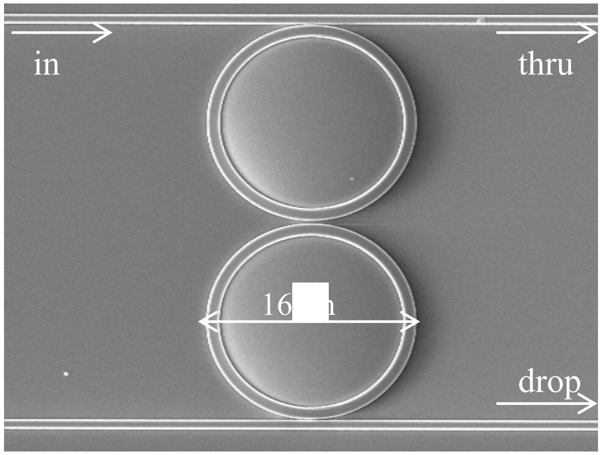
- Form discretized EFIE matrix M with imaginary k
  - Integral Operator has exponentially decaying REAL kernel.
  - Must compute for many values of k.
- Compute logdet(M * Minf $^{-1}$) or trace(M $^{-1}$ dM/dz) and sum over k
  - Fast methods (e.g. PFFT) form matrix-vector products quickly.
  - Iterative methods for f(matrix) a newer area.
  - Investigate fast inverse representations?



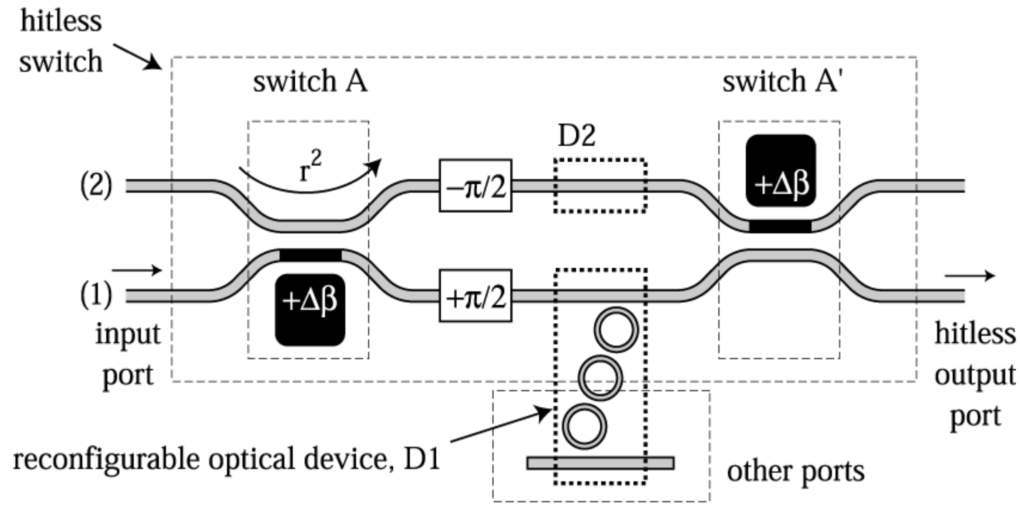
Results: Non-monotonic dependence of force on sidewall separation (3D)



Growing Variety of Nanophotonic Applications

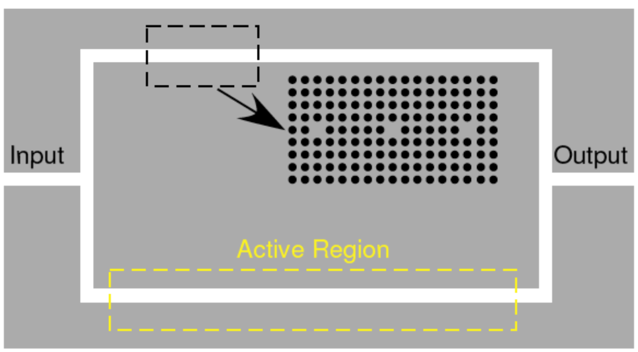


Ring Resonator (Thanks CIPS at MIT)

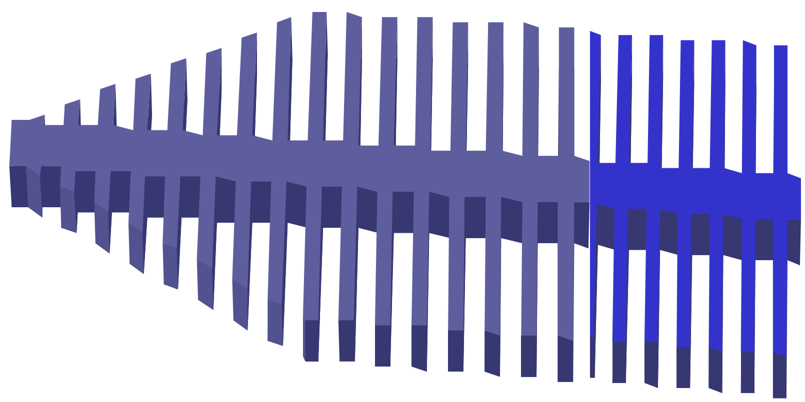


(a)

Optical Switch (Thanks CIPS at MIT)

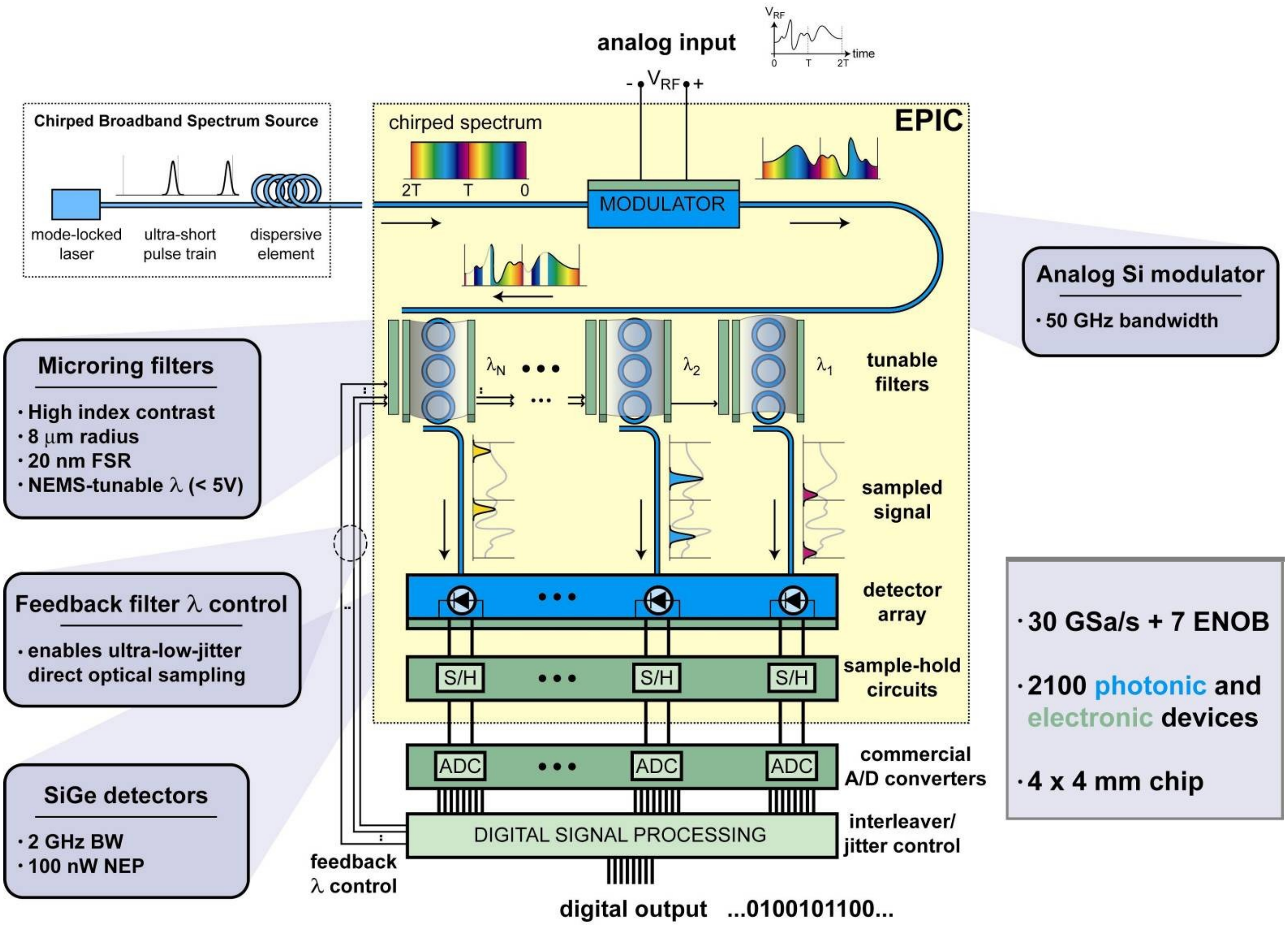


Mach-Zehnder Interferometer (thanks S. Johnson)



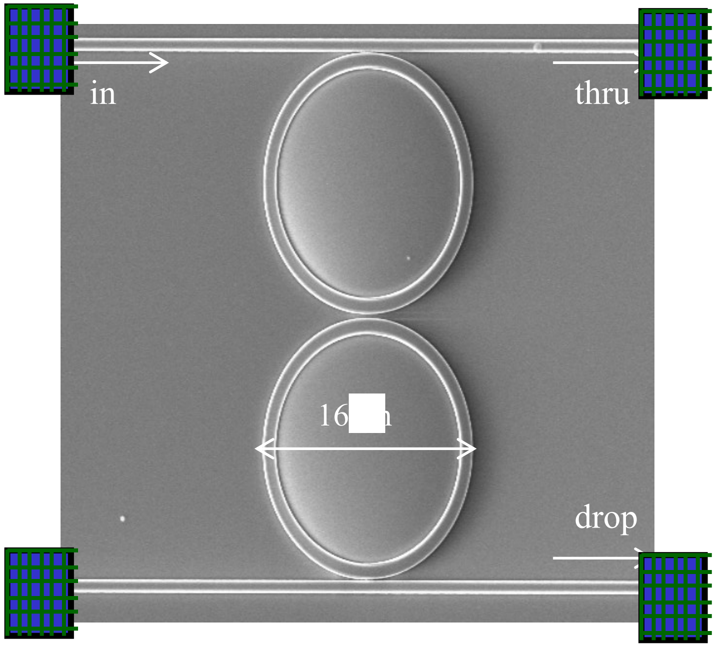
Slow light wave guide with coupler

Photonic/Electronic System (Slide Thanks To CIPS)



CIPS AT MIT

Need Absorbers for Photonics



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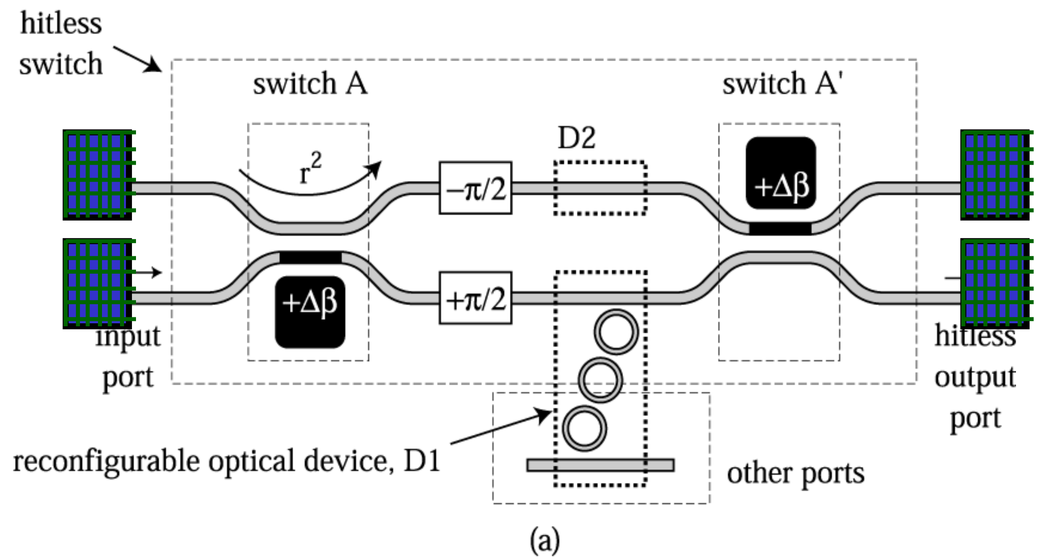

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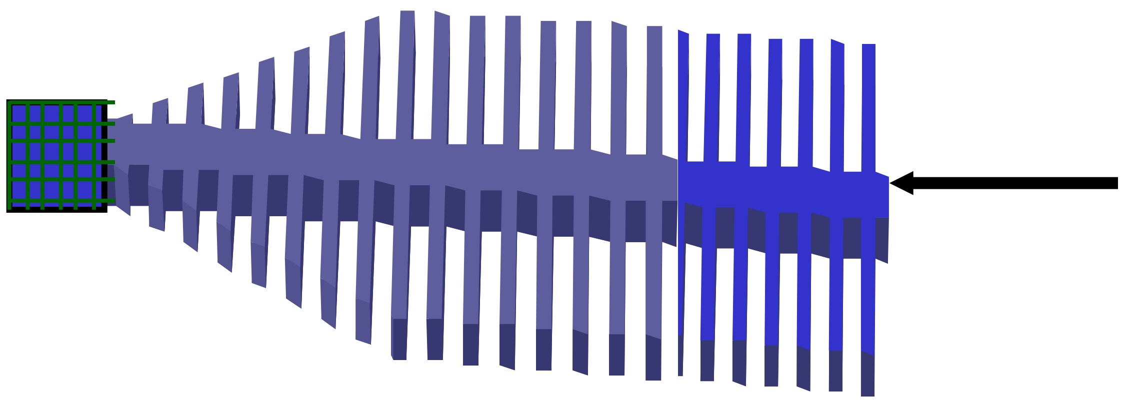
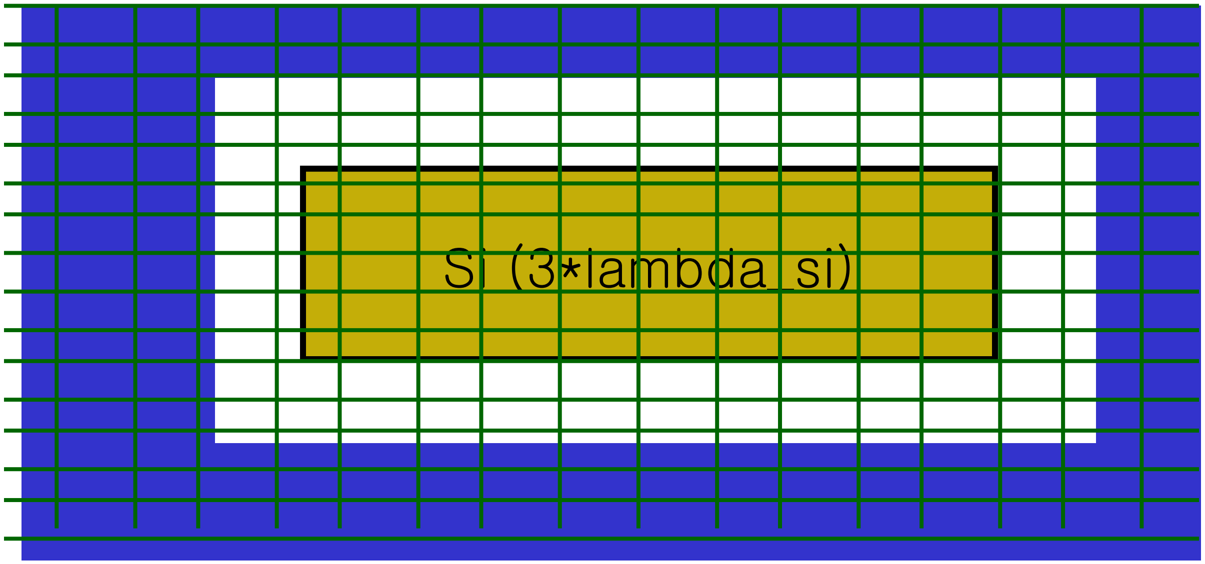


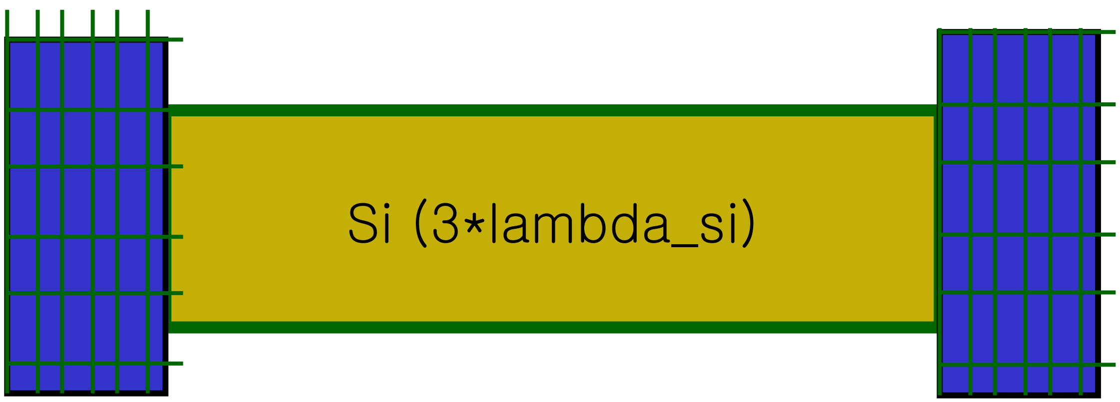
Geometry Matched Absorber

Slow Light Coupler

Absorbers for Photonics

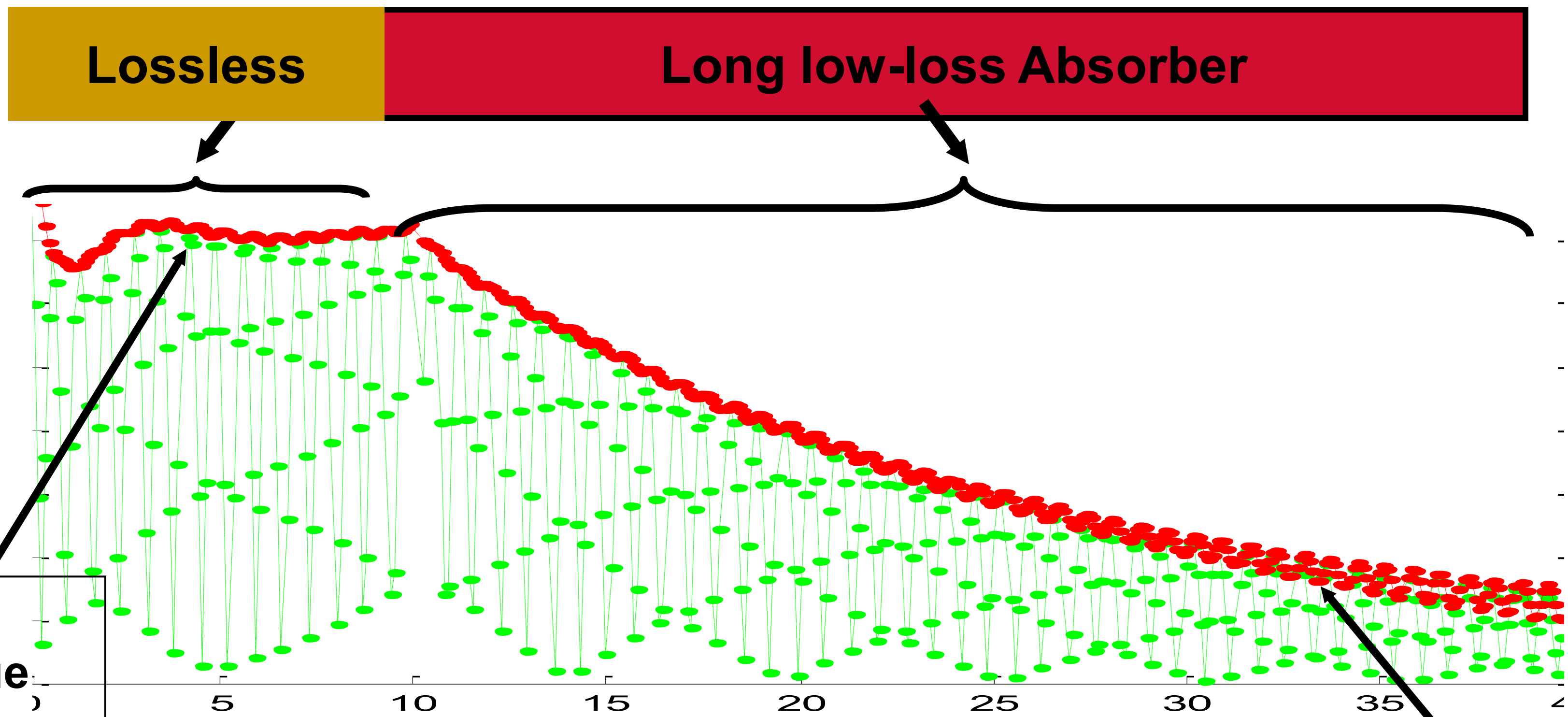


FD/ FEM solvers,
-having a much larger computational domain



Fast Integral Equation Solvers

Straightforward Approach

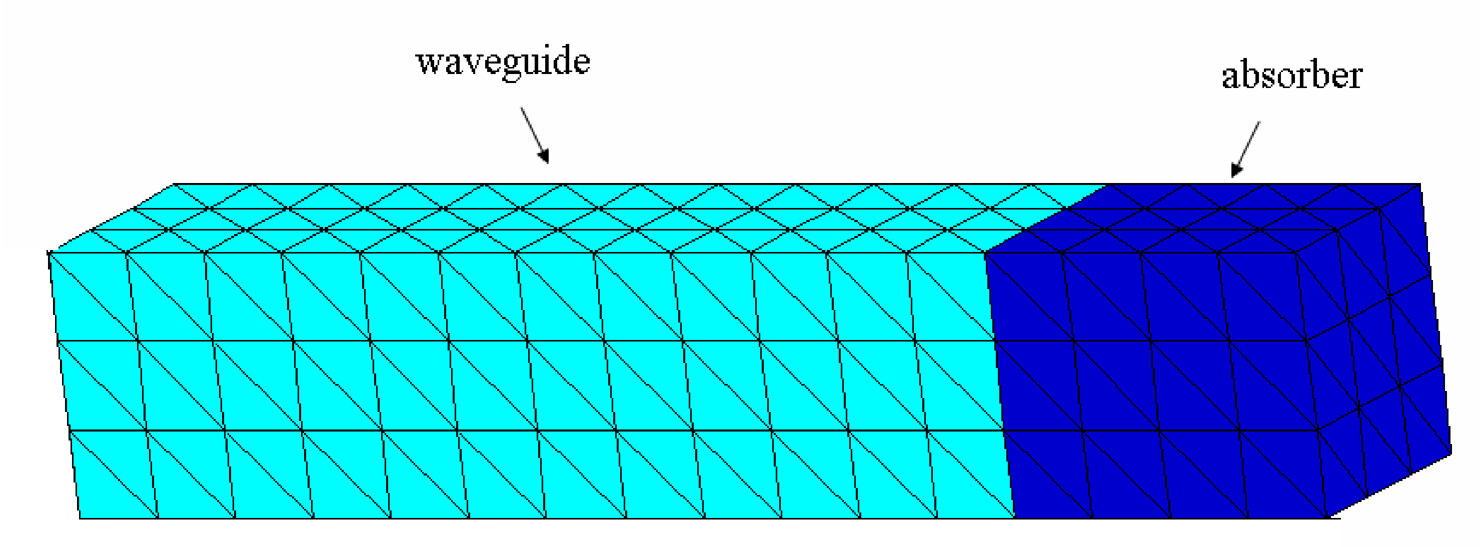


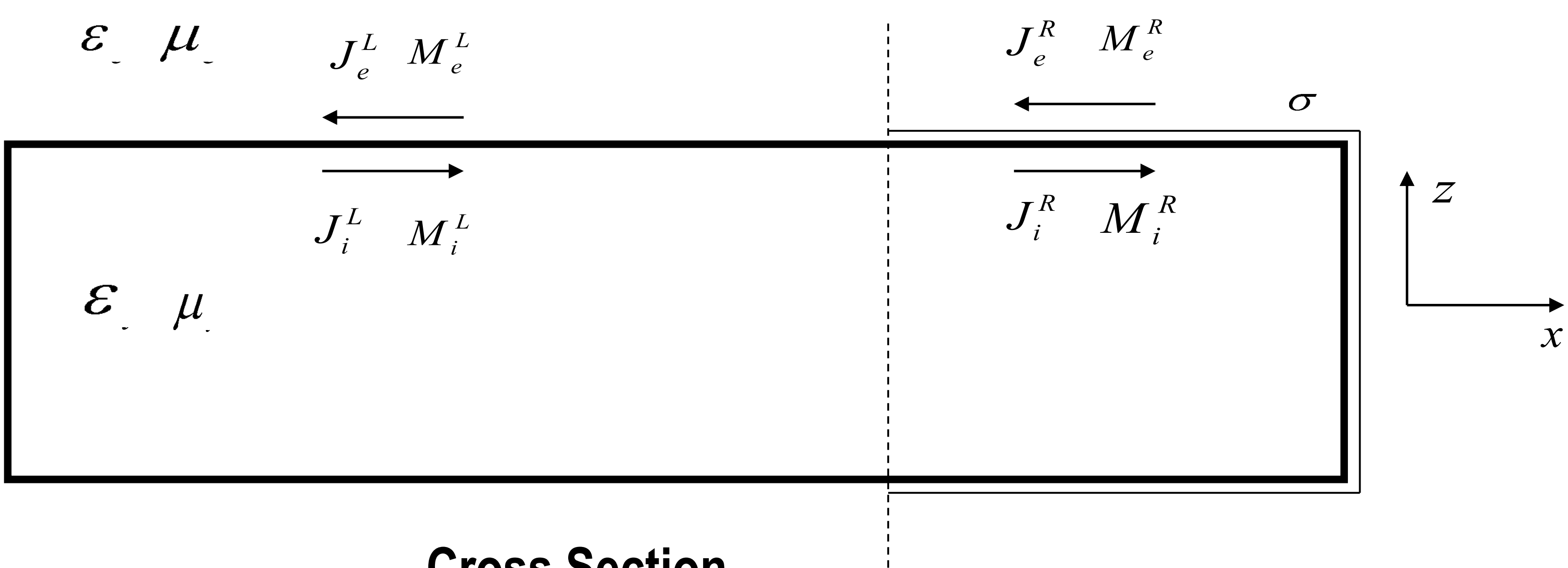
Smaller ripples due to near zero reflections very low loss, long absorber

Reflected wave dissipates in long absorber before effecting device

- Fast long low-loss absorber (3-D)
  - Extremely fast circulently preconditioned Toeplitz solver
  - 40 Wavelengths < 1 hour
    - Slow setup (matlab prototype)
    - Solve portion under 30 seconds!
  - Works on general fast code

Novel Surface Absorber





Cross Section

Surface Absorber Formulation

Modified PMCHW formulation to incorporate the electrical conductance on the absorber surface

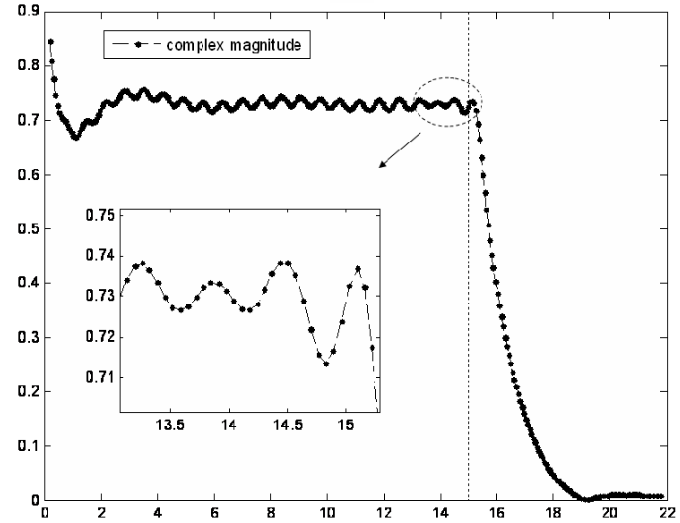
$$\hat{n} \times [\mathbf{E}^R_{inc} + \mathbf{E}^R_e(\mathbf{J}^L_e, \mathbf{M}^L_e, \mathbf{J}^R_e, \mathbf{M}^R_e)] = \hat{n} \times [\mathbf{E}^R_i(\mathbf{J}^L_i, \mathbf{M}^L_i, \mathbf{J}^R_i, \mathbf{M}^R_i)],$$

$$\hat{n} \times [\mathbf{H}^R_{inc} + \mathbf{H}^R_e(\mathbf{J}^L_e, \mathbf{M}^L_e, \mathbf{J}^R_e, \mathbf{M}^R_e) - \mathbf{H}^R_i(\mathbf{J}^L_i, \mathbf{M}^L_i, \mathbf{J}^R_i, \mathbf{M}^R_i)] = \sigma \mathbf{E}^R_{tan}$$

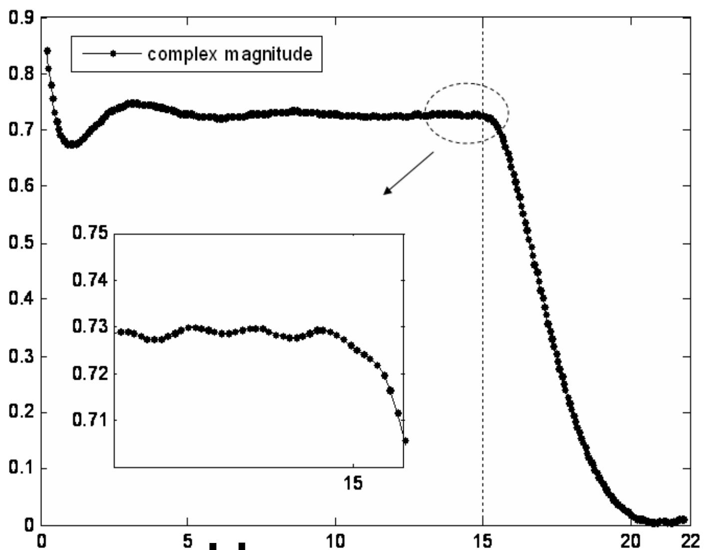
- **The tangential electrical field is continuous**
- **The tangential magnetic field has a jump due surface currents through the surface conductivity.**

Effects of Surface Conductance Profile

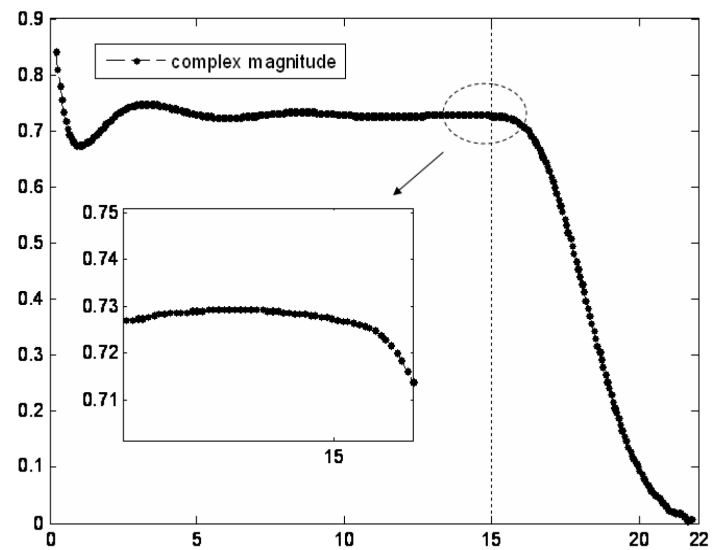
Field pattern (complex magnitude) along waveguide by different surface conductance profile



Constant



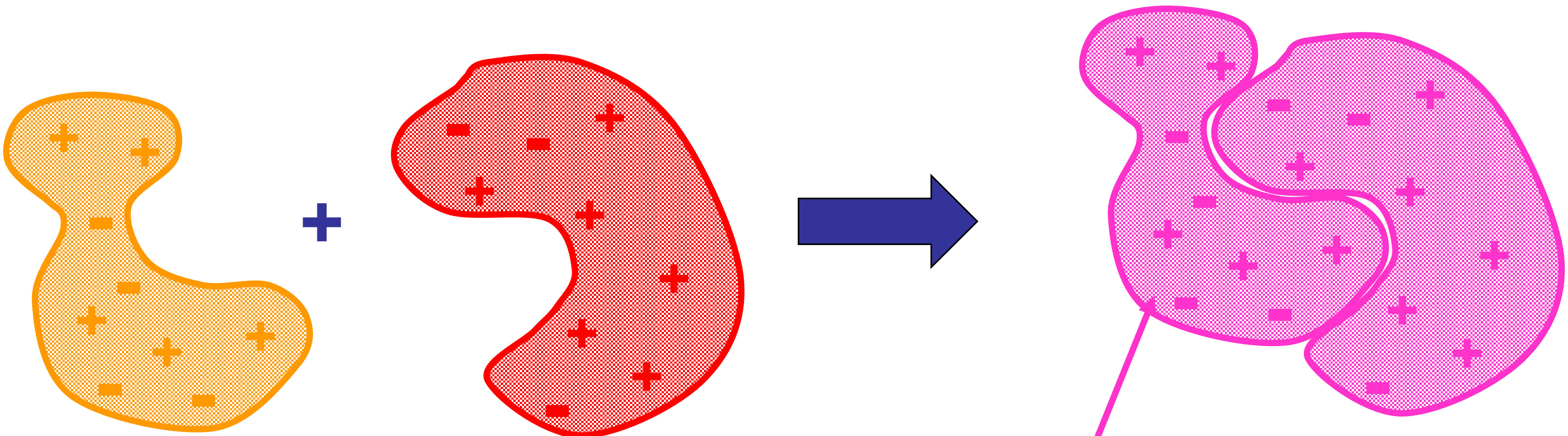
Linear



Quadratic

Drug Design Problem - Minimize Electrostatic Binding Energy

$$E_{binding} = \qquad + \qquad -$$

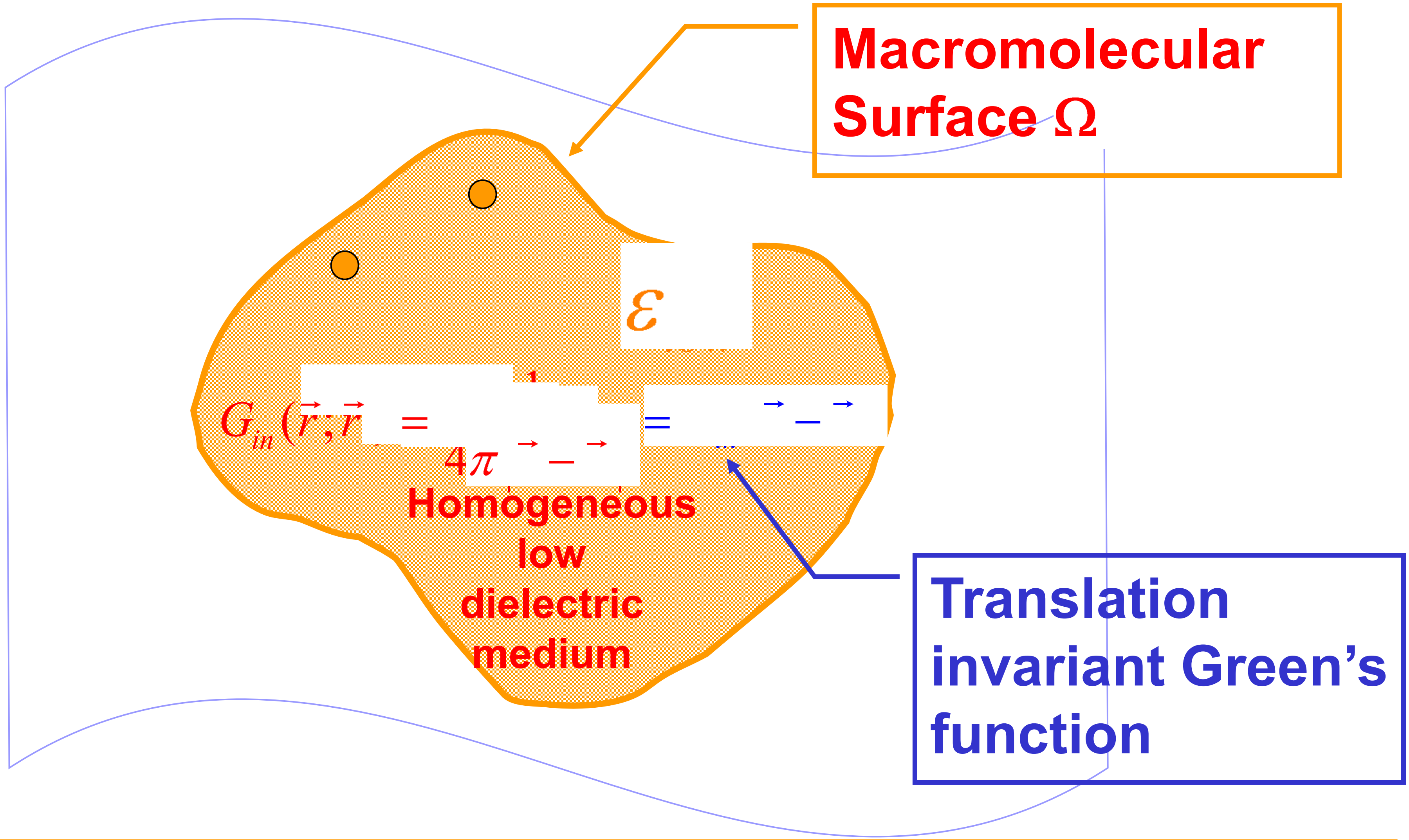


Higher energy

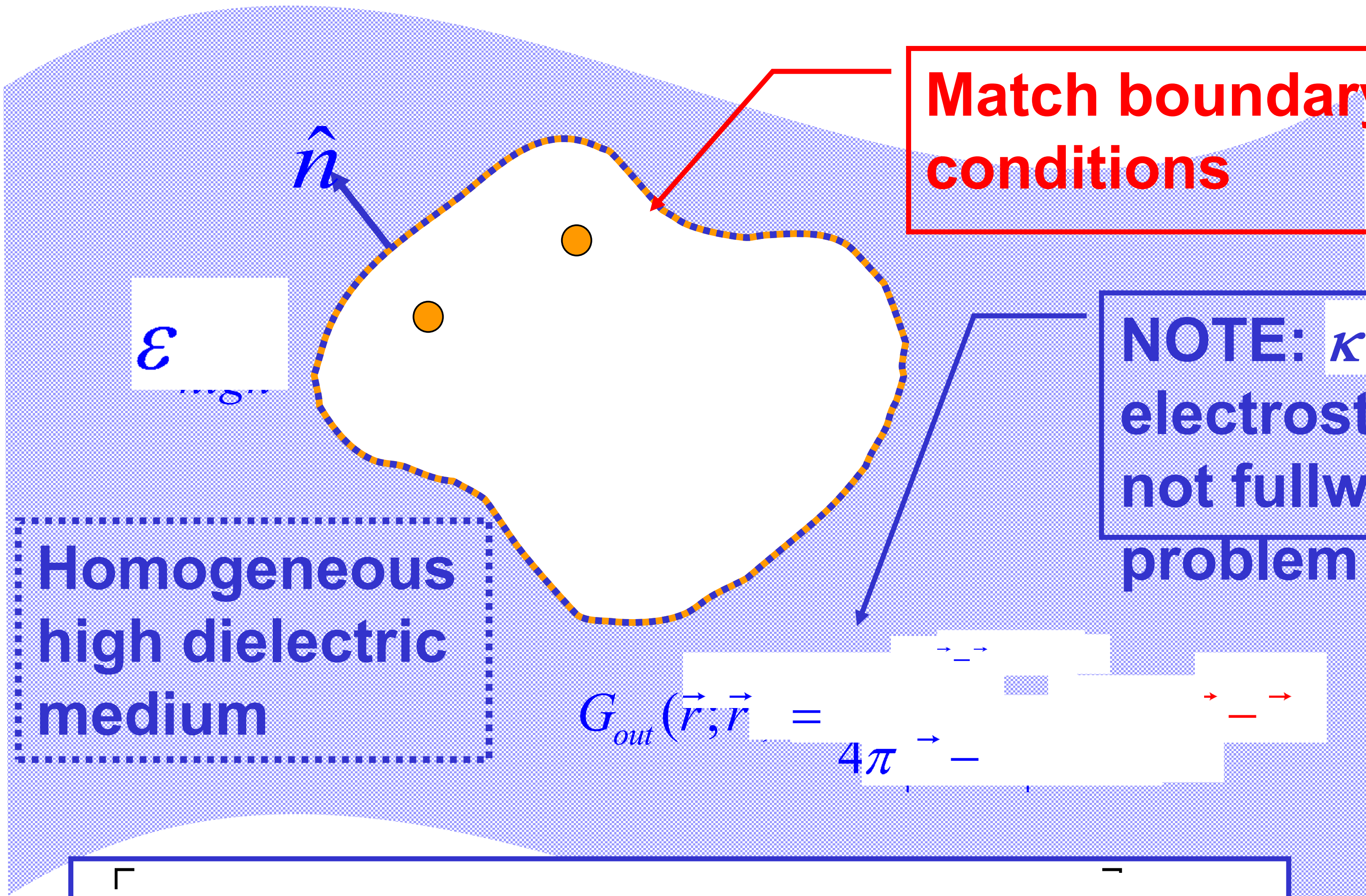
Lower energy

Determine the charge distribution in the ligand so that it is "Energetically Optimized" to bind

Integral equation: Interior Problem



Integral equation: Exterior Problem



$\int_{\Omega} \left[\cdots \right]$

φ_{in}

$\frac{1}{\varepsilon} \frac{\partial}{\partial}$

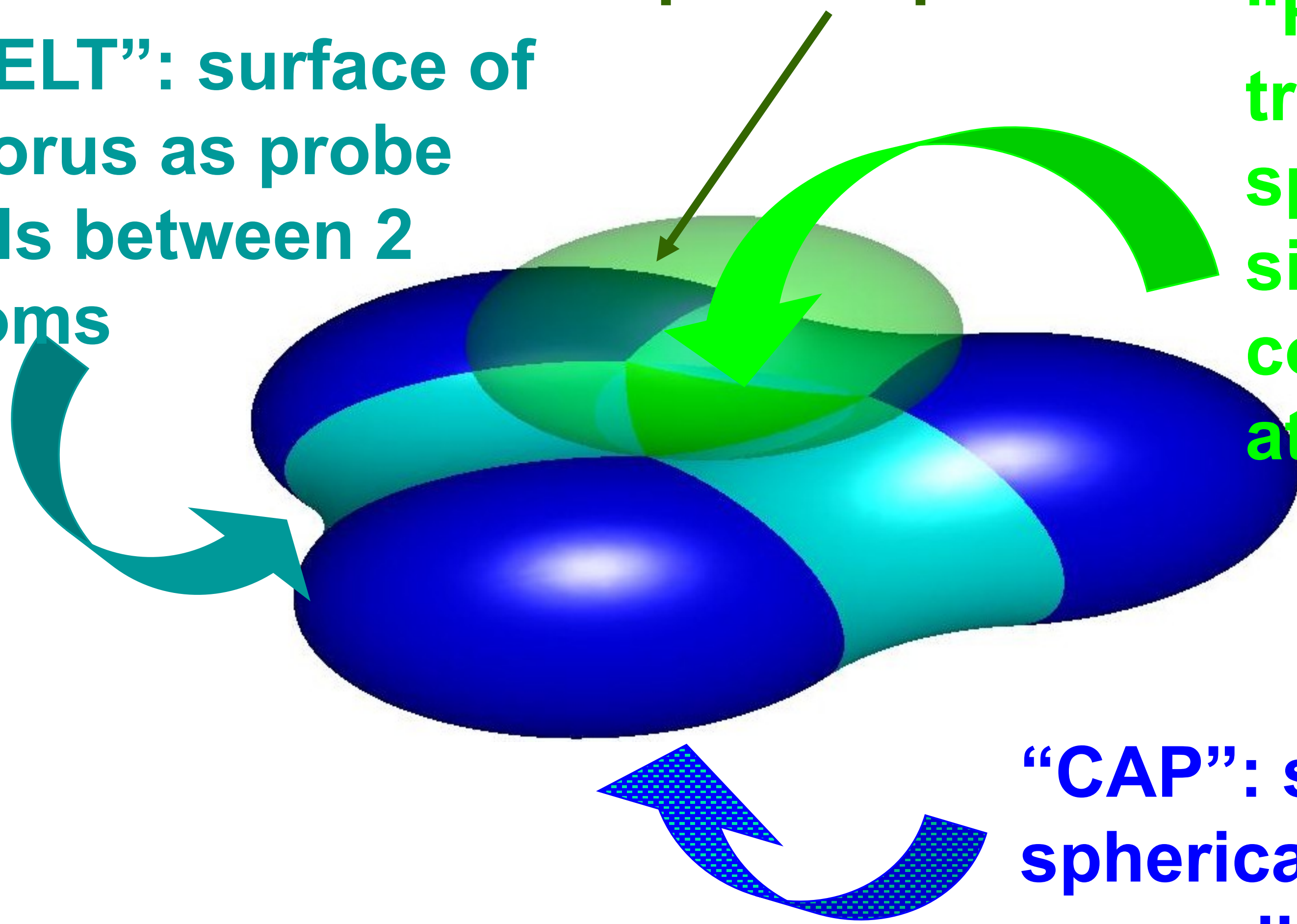
Molecular Surface Representation

Molecule made up of spherical atoms
Molecular surface generated by a rolling probe

probe sphere

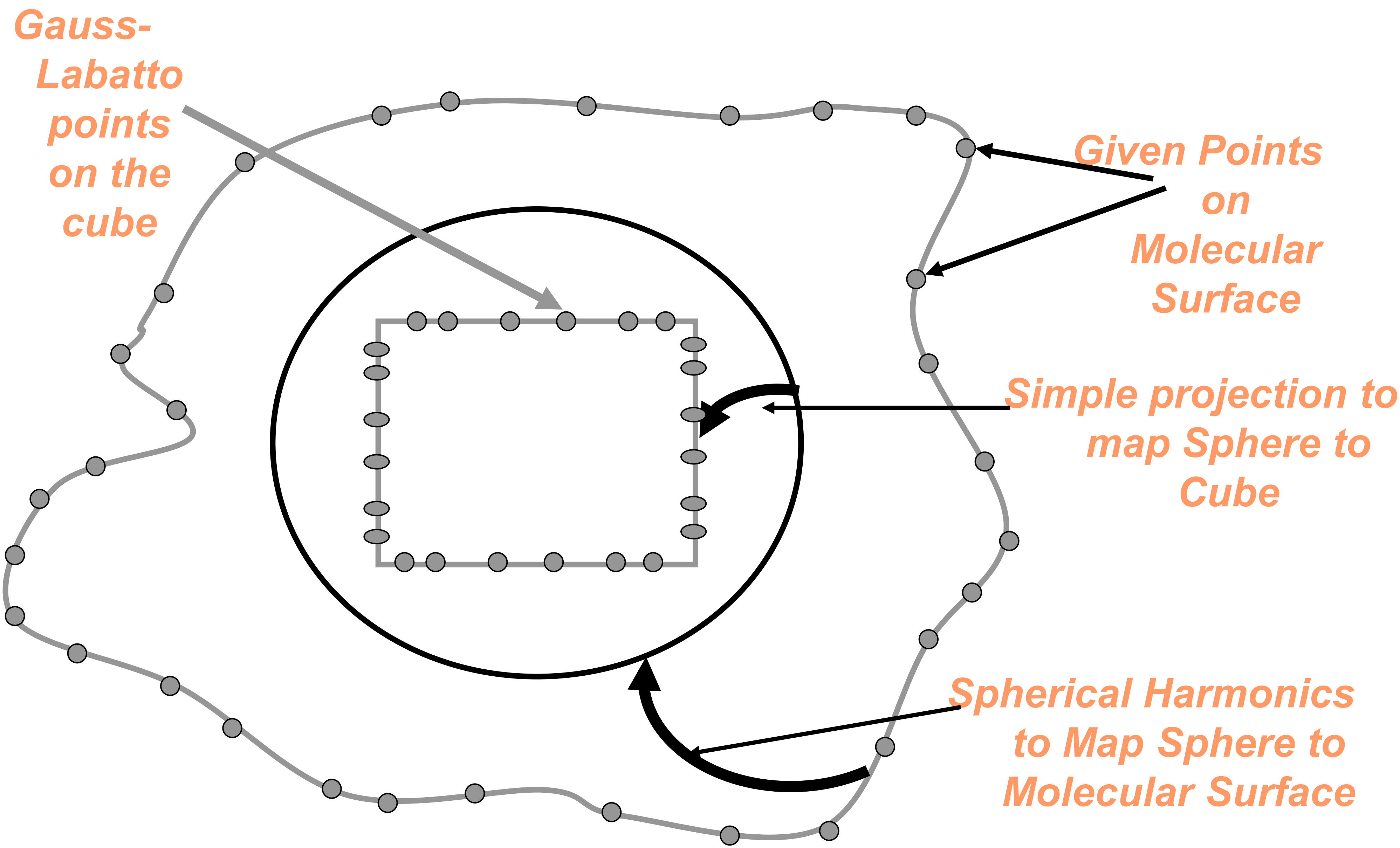
"BELT": surface of a torus as probe rolls between 2 atoms

"PIT": spherical triangle on probe sphere when simultaneously in contact with 3 atoms

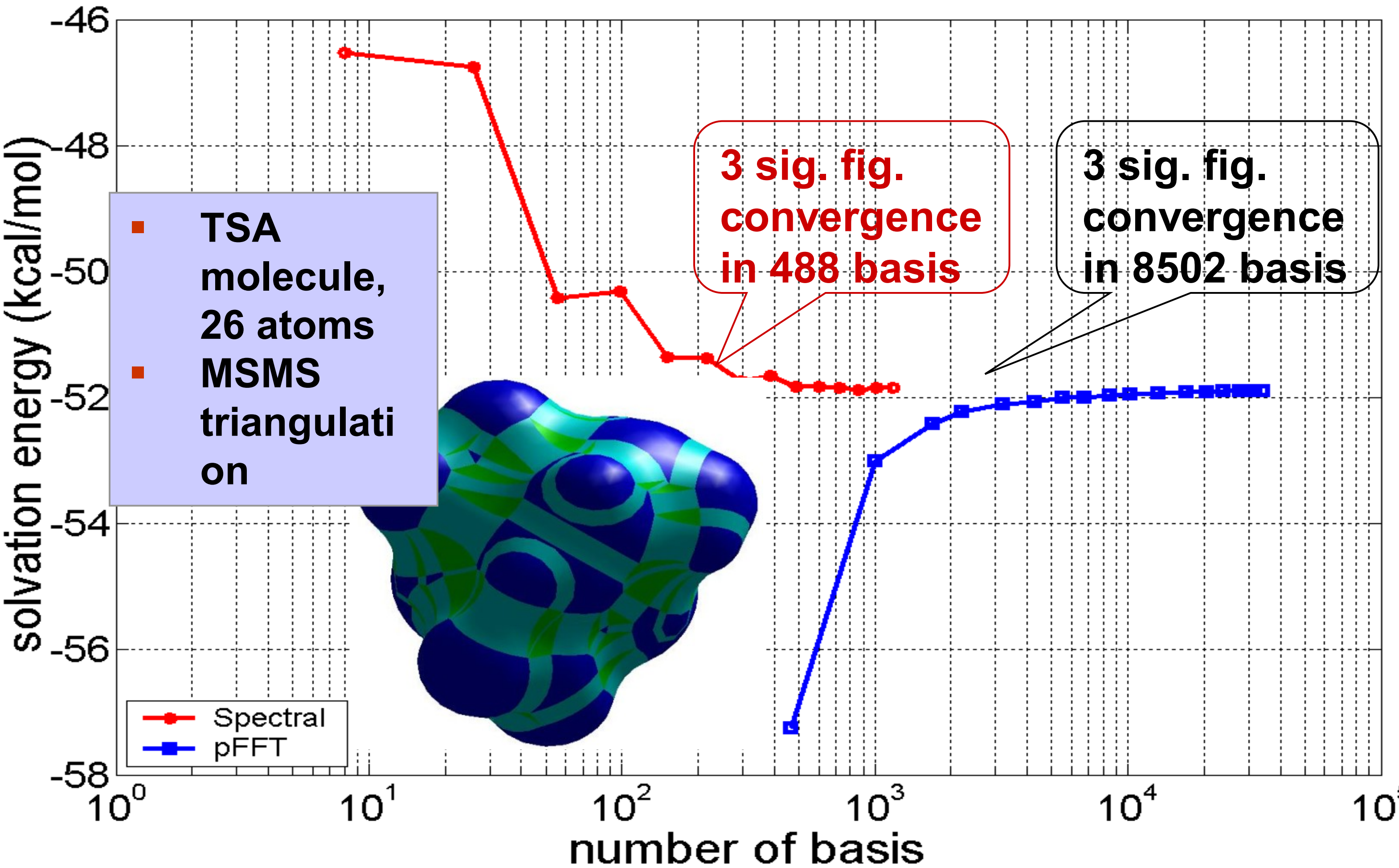


"CAP": surface of spherical atoms accessible by probe

"Meshless" Approach by Picture



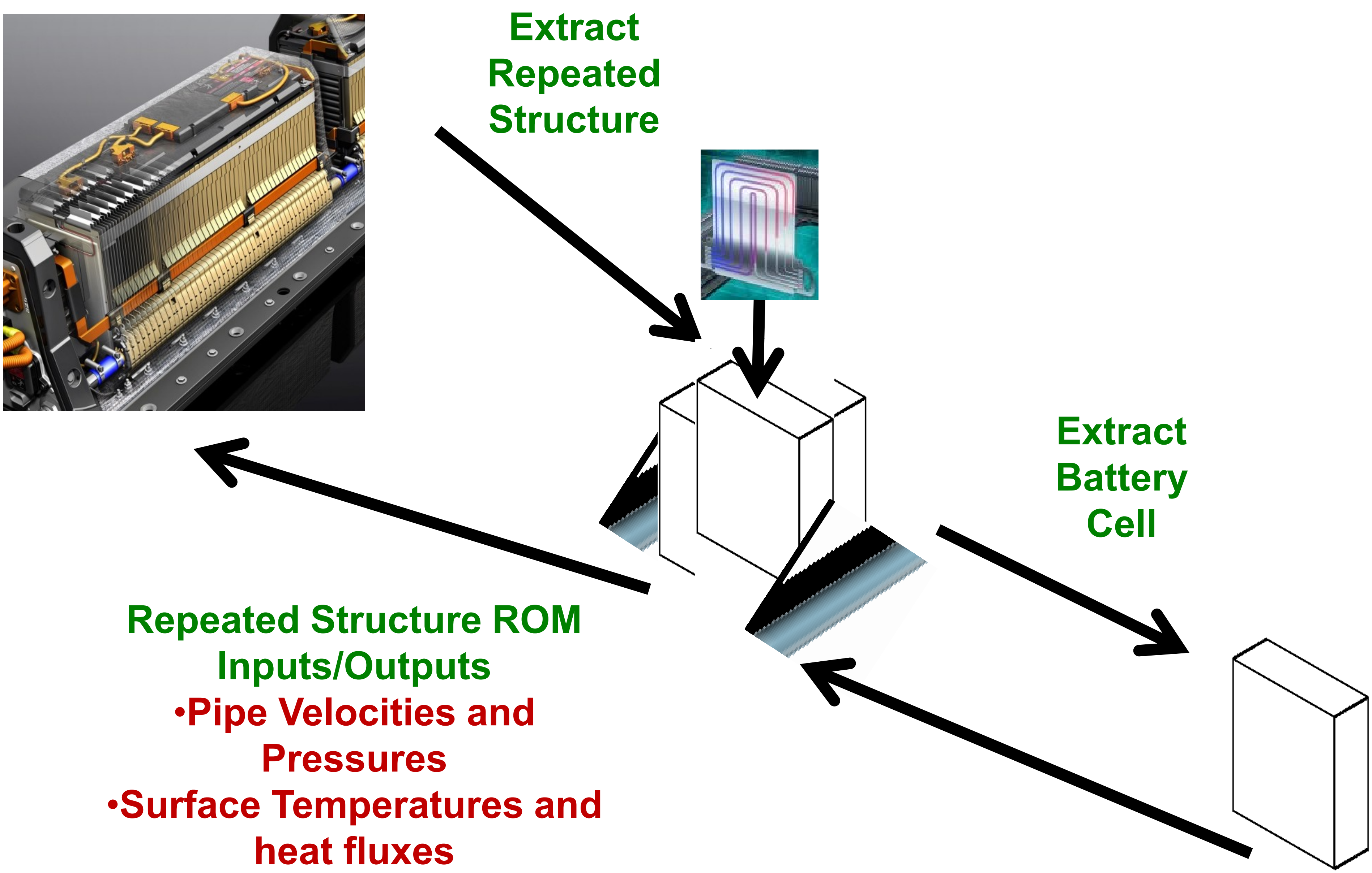
Higher Order Meshless Method For Molecular Surfaces



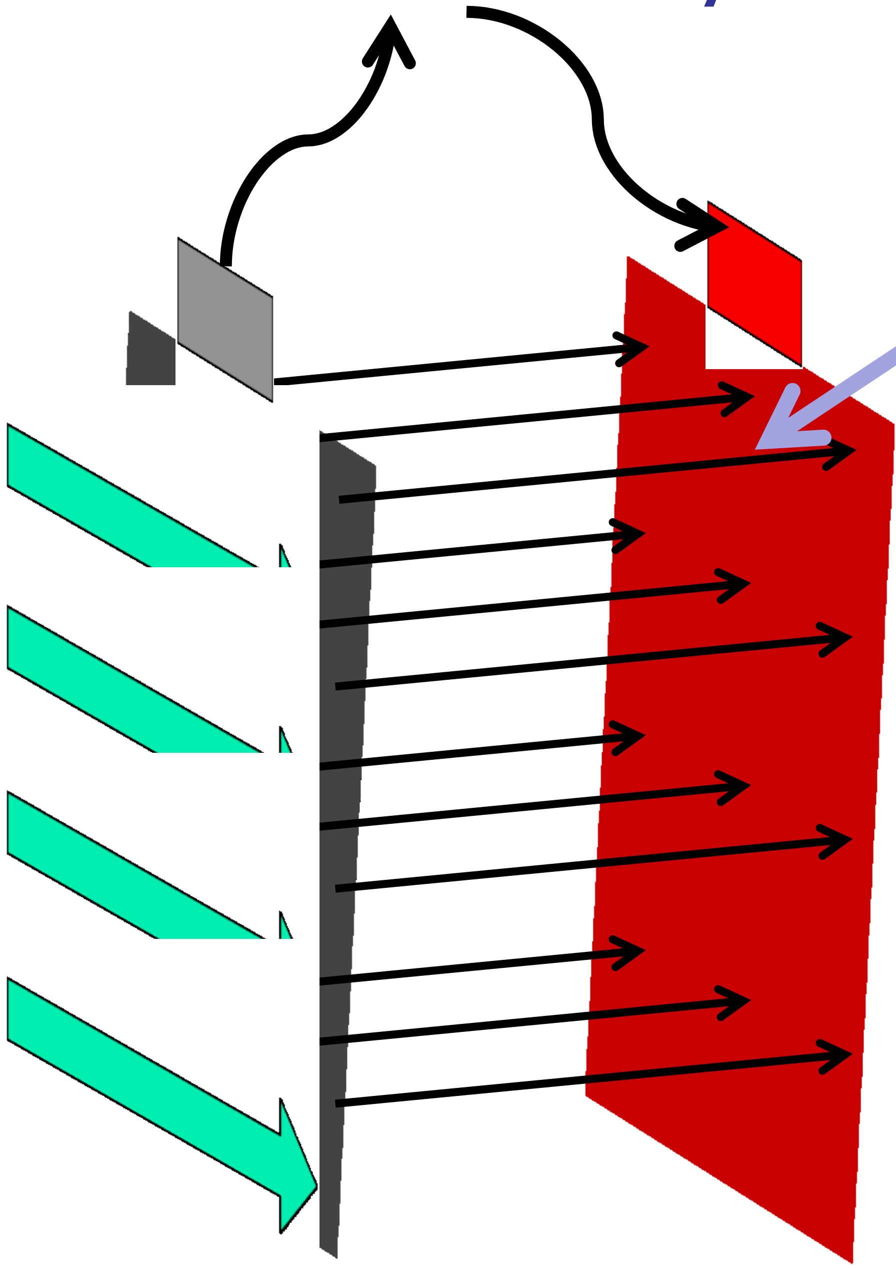
- Flat-panel versus higher-order + meshless
- Coupled Poisson, Possion-Boltzmann Equation
- CPU Time < Hour (Matlab Prototype)
- S. Kuo

- Limited Impact on biological computations.

Multiphysics Example – Battery Packs



Cooled Battery with 1-D Electrochem Model



- NTGK Electrochemistry model

$$i = f(\phi_+ - \phi_-, DOD)$$
$$\frac{d}{dt}DOD = f(\phi_+ - \phi_-, DOD)$$

- Electrical Conductivity Model

$$\sigma_e \nabla^2 \phi_+ = i$$
$$\sigma_e \nabla^2 \phi_- = -i$$

- Thermal Conductivity Model

$$\sigma \nabla^2 T = (\phi_+ - \phi_-) * i$$

- Sheet Flow Model

$$\sigma_s \nabla^2 T_s + MFR \cdot \nabla T_s = \alpha \cdot (T_s - T)$$

Linearized Systems

- Fluids (descriptor)
  - Pressure-Velocity

$$\frac{d}{dt}M\vec{x}(t) = A\vec{x}(t) + B\,\vec{u}(t)$$
$$y(t) = C\vec{x}(t) + D\vec{u}(t)$$

- Mech (2nd Order)
  - Force-Displacement

$$M\frac{d^2}{dt^2}\vec{x}(t) = F\frac{d}{dt}\vec{x}(t) + K\vec{x}(t) + B\,\vec{u}(t)$$
$$y(t) = C\vec{x}(t) + D\vec{u}(t)$$

- Electromag (frequency dependent)

$$\omega^2 A(j\omega)\vec{x}(j\omega) + j\omega F(j\omega)\vec{x}(j\omega) + K(j\omega)\vec{x}(j\omega) + B(j\omega)\,\vec{u}(j\omega) = 0$$

  - Currents-Voltages

$$y(j\omega) = C(j\omega)\vec{x}(j\omega) + D(j\omega)\vec{u}(j\omega)$$

Projection Framework

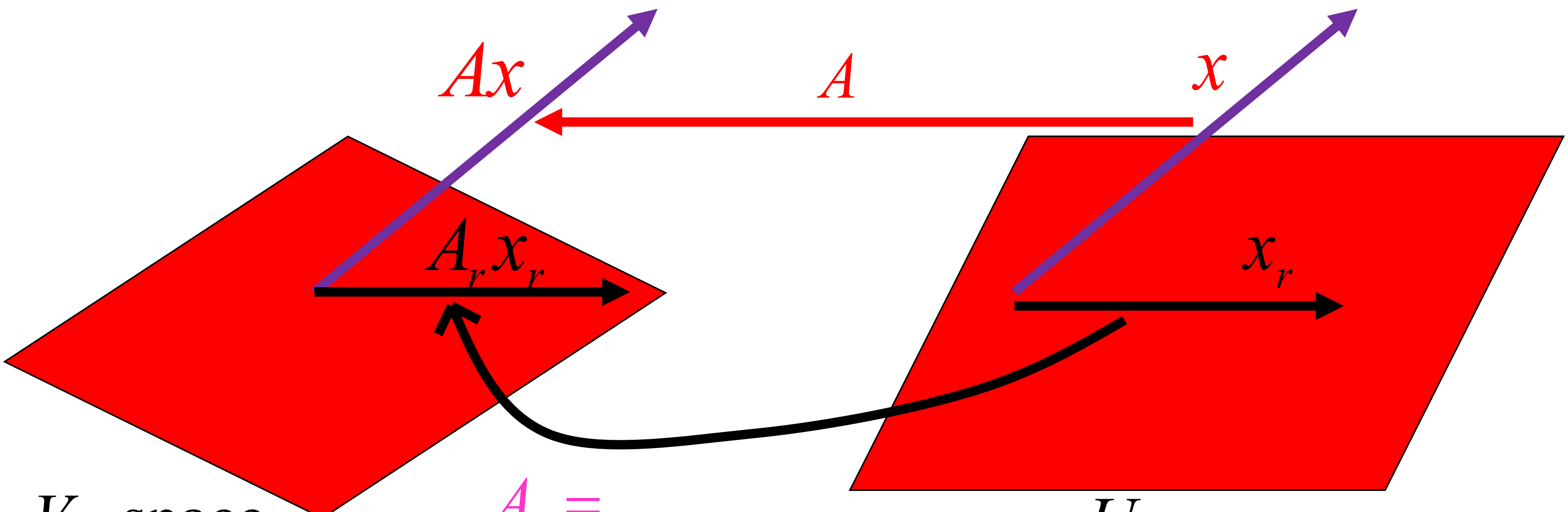
$$\dot{x} = Ax + bu,\ \ y = c^T x \ \Rightarrow \dot{x}_r = A_r x_r + b_r u,\ \ y_r = c_r^{\ T} x$$

Equation Testing

$V_q^{\ T} Ax \approx$

Change of variables

$x \approx$



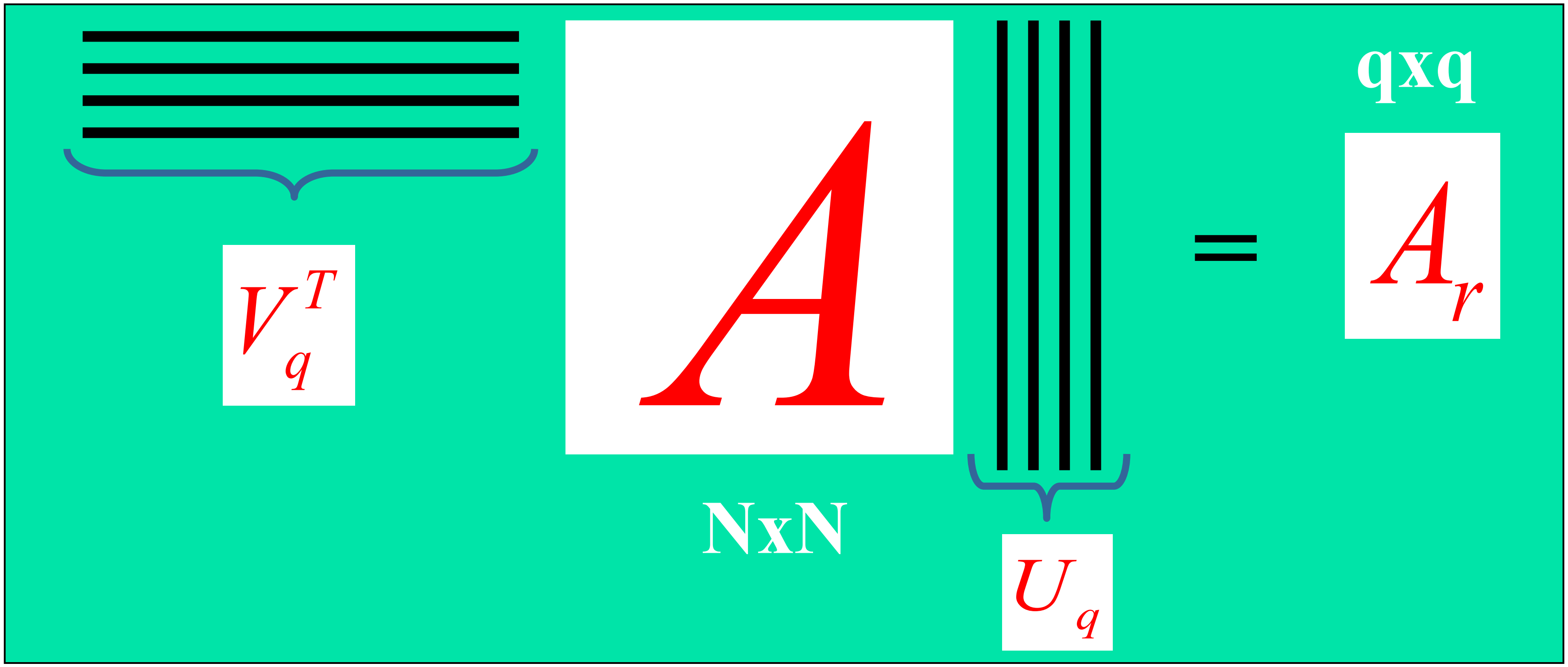
V_q space

$A_r =$

U_q space

Galerkin $\rightarrow$ ce $= U_q$ space

Forming the Reduced Matrix



- No explicit A need, Only Matrix-vector products

  For each column of U_q

  Multiply by A, then dot result with columns of V_q

Projection For Descriptor Systems

$$M\frac{dx}{dt} = Ax + Bu$$
$$y = Cx + Du$$

$$V_q^T M U_q \frac{dx_r}{dt} = V_q^T A U_q x_r + V_q^T B u$$
$$y = C U_q x_r + Du$$

$$M_r \frac{dx_r}{dt} = A_r x_r + B_r u$$
$$y = C_r x_r + Du$$

where

$$M_r = V_q^T M U_q$$
$$A_r = V_q^T A U_q$$
$$B_r = V_q^T B$$
$$C_r = C U_q$$

Picking U and V

- Use Eigenvectors (Modes)
- Use Time Series Data (Snapshot Method, POD)
  - Use the SVD to pick *q* < *k* important vectors

$$x\ \ t_0\ \ , x\ \ t_1\ \ , \cdots$$

- Use Frequency Domain Data (Freq. Domain POD, PMTBR)
  - Use the SVD to pick *q* < *k* important vectors

$$X\ \ s_1\ \ , X\ \ s_2\ \ , \cdots$$

- Krylov subspace Vectors
  - Again use SVD to pick q < k important vectors
- Use Singular Vectors of System Grammians (Too Costly)

Krylov For Fluids and Mech

- Standard Krylov Subspace

$$span\{A^{-1}B, A^{-2}B, A^{-3}B, ..., A^{-k}B\}$$

  - Must back orthogonalize at each step

- Krylov for Descriptor Systems with Singular M

$$span\{A^{-1}MA^{-1}B, (A^{-1}M)^2 A^{-1}B, (A^{-1}M)^3 A^{-1}B, ... (A^{-1}M)^k A^{-1}B\}$$

  - Still must back orthogonalize at each step

- Krylov for Mech $M \leftarrow \begin{pmatrix} I & 0 \\ 0 & M \end{pmatrix} \quad A \leftarrow \begin{pmatrix} 0 & I \\ K & F \end{pmatrix}$

$$span\{A^{-1}MA^{-1}B, (A^{-1}M)^2 A^{-1}B, (A^{-1}M)^3 A^{-1}B, ... (A^{-1}M)^k A^{-1}B\}$$

  - Only Keep Top Half of the vectors

Problems with MOR for nonlinear

- **Sub:** $x = Vz$ **to** $\frac{dx}{dt} = f(x) + Bu$

- **Reduced system:** $$\frac{dz}{dt} = \overbrace{V^T f(Vz)}^{\hat{f}(z)} + V^T Bu$$

- **Problem:** $W^T f(Vz) : \underset{\text{small}}{R^q} \rightarrow \underset{\text{large}}{R^N} \rightarrow \underset{\text{large}}{R^N} \rightarrow \underset{\text{small}}{R^q}$

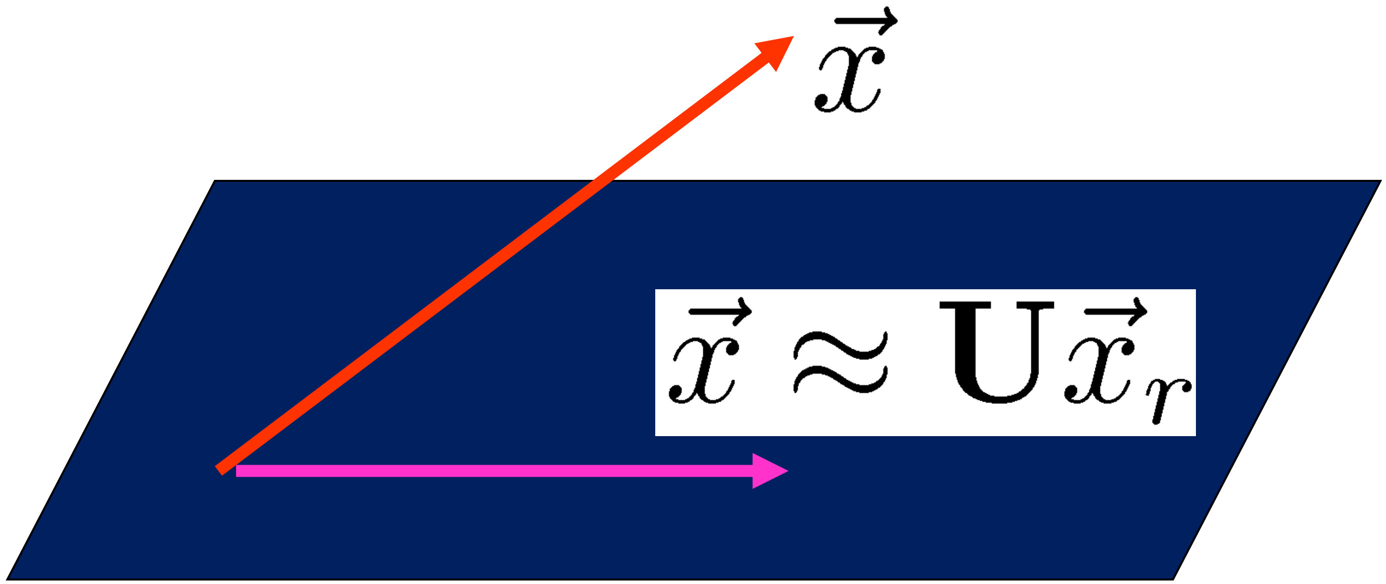
  $q=10 \qquad N=10^4 \qquad N=10^4 \qquad q=10$

- **Using $W^T f(Vz)$ is too expensive!**

Projection Assumption 1

- For all inputs of interest

$$x(t) \approx\in span\{\vec{U}_1\ \vec{U}_2 \ldots \vec{U}_q\}\ \ q << n$$



- U's could be generated from
  - SVD of time series data,
  - Krylov subspaces from linearizations, etc.

Projection Assumption 2

- There is a space: $\mathbf{V} = \{\vec{V}_1, ..., \vec{V}_q\}$ such that:
- ***If*** the residual is forced orthogonal to $\mathbf{V}$

$$\vec{r}(t) \equiv \frac{d}{dt}\mathbf{U}\vec{x}_r(t) - \left(f\left(\mathbf{U}\vec{x}_r(t)\right) + \vec{b}\, u(t) \right)$$

with $\vec{x}_r(t)$ such that $\mathbf{V}^T \vec{r}(t) = 0$

- ***Then*** the U-restricted DE is almost satisfied

$$\vec{r}(t) \equiv \frac{d}{dt}\mathbf{U}\vec{x}_r(t) - \left(f\left(\mathbf{U}\vec{x}_r(t)\right) + \vec{b}\, u(t) \right) \approx 0$$

U = V a common choice

- In General

$$\mathbf{V}^T\mathbf{U}\frac{d}{dt}\vec{x}_r(t) = \mathbf{V}^T f\left(\mathbf{U}\vec{x}_r(t)\right) + \mathbf{V}^T\vec{b}\,z(t)$$

- If U = V and U^T U = I

$$\frac{d}{dt}\vec{x}_r(t) = \mathbf{U}^T f\left(\mathbf{U}\vec{x}_r(t)\right) + \mathbf{U}^T\vec{b}\,z(t)$$

- Good for systems from self-adoint PDE's:
  - Spatial discretization of nonlinear heat conduction

$$\frac{\partial}{\partial t}\vec{x}(t) = \nabla\cdot f\left(\nabla\vec{x}(t)\right) + \vec{b}\;\; z(t)$$

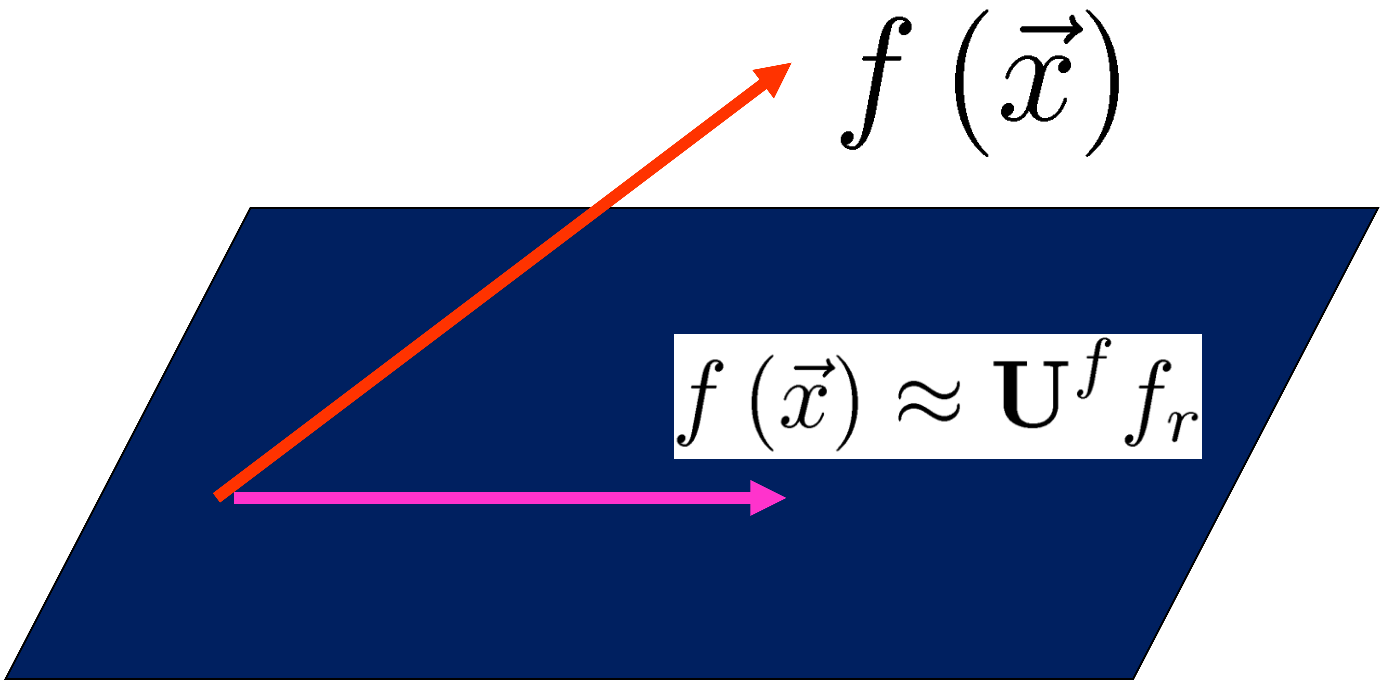
  - Spatial discretization of the Poisson-Boltzmann

$$\frac{\partial}{\partial t}\vec{x}(t) = \nabla^2 x\vec{(t)} + f\left(\vec{x}(t)\right) + \vec{b}\;\; z(t)$$

Assumption 3 (For DEIM)

- For x's generated by all inputs of interest

$$f\left(x(t)\right) \approx \in span\{\vec{U}_1^f \; \vec{U}_2^f \ldots \vec{U}_q^f\} \;\; q << n$$



Assumption 3 Implies:

- We can replace "Galerkin"

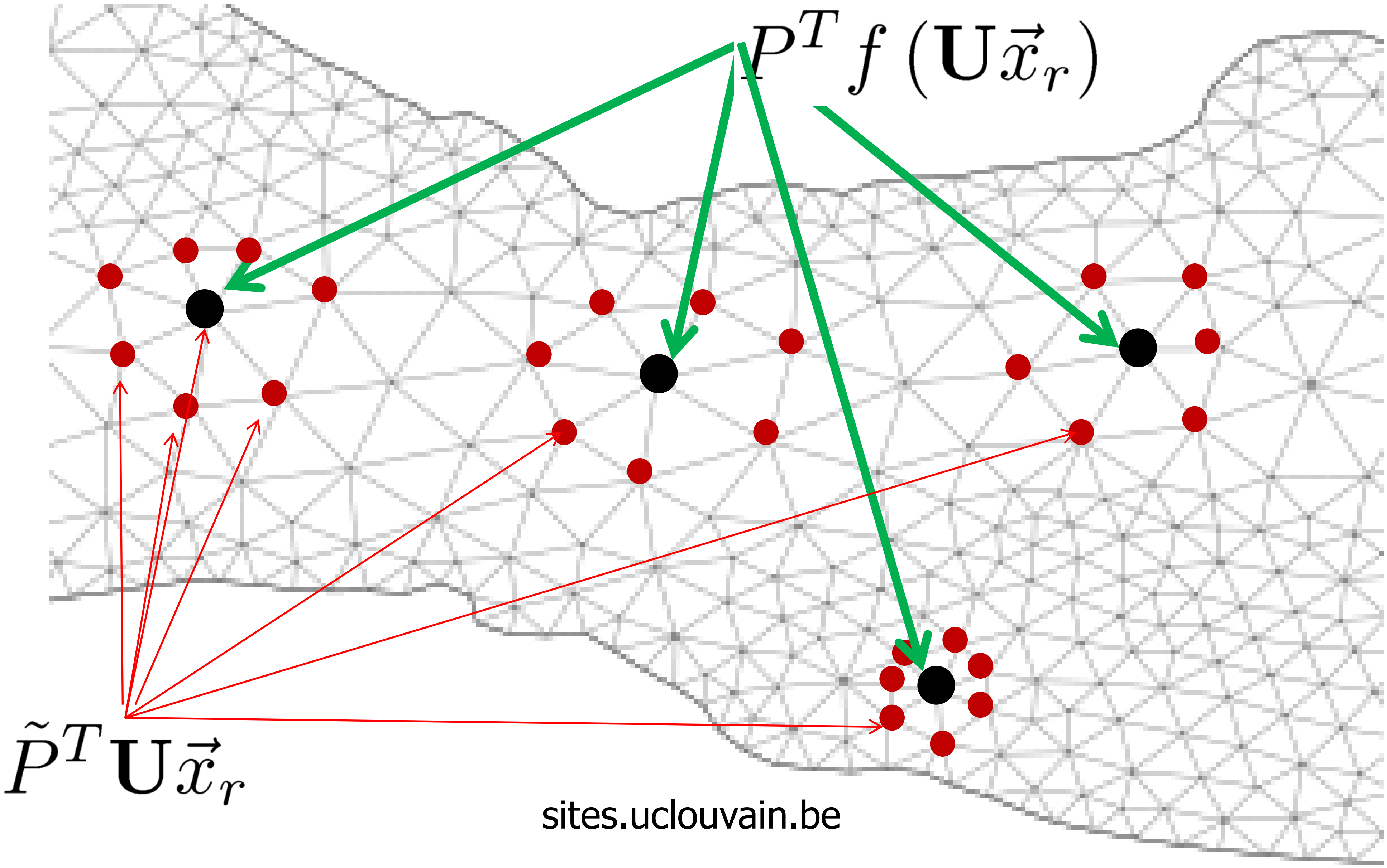
$$f_r = \left(\mathbf{U}^f\right)^T f\left(\mathbf{U}\vec{x}_r\right)$$

- With "Gappy Collocation"

$$P^T \mathbf{U}^f f_r = P^T f\left(\mathbf{U}\vec{x}\right)$$

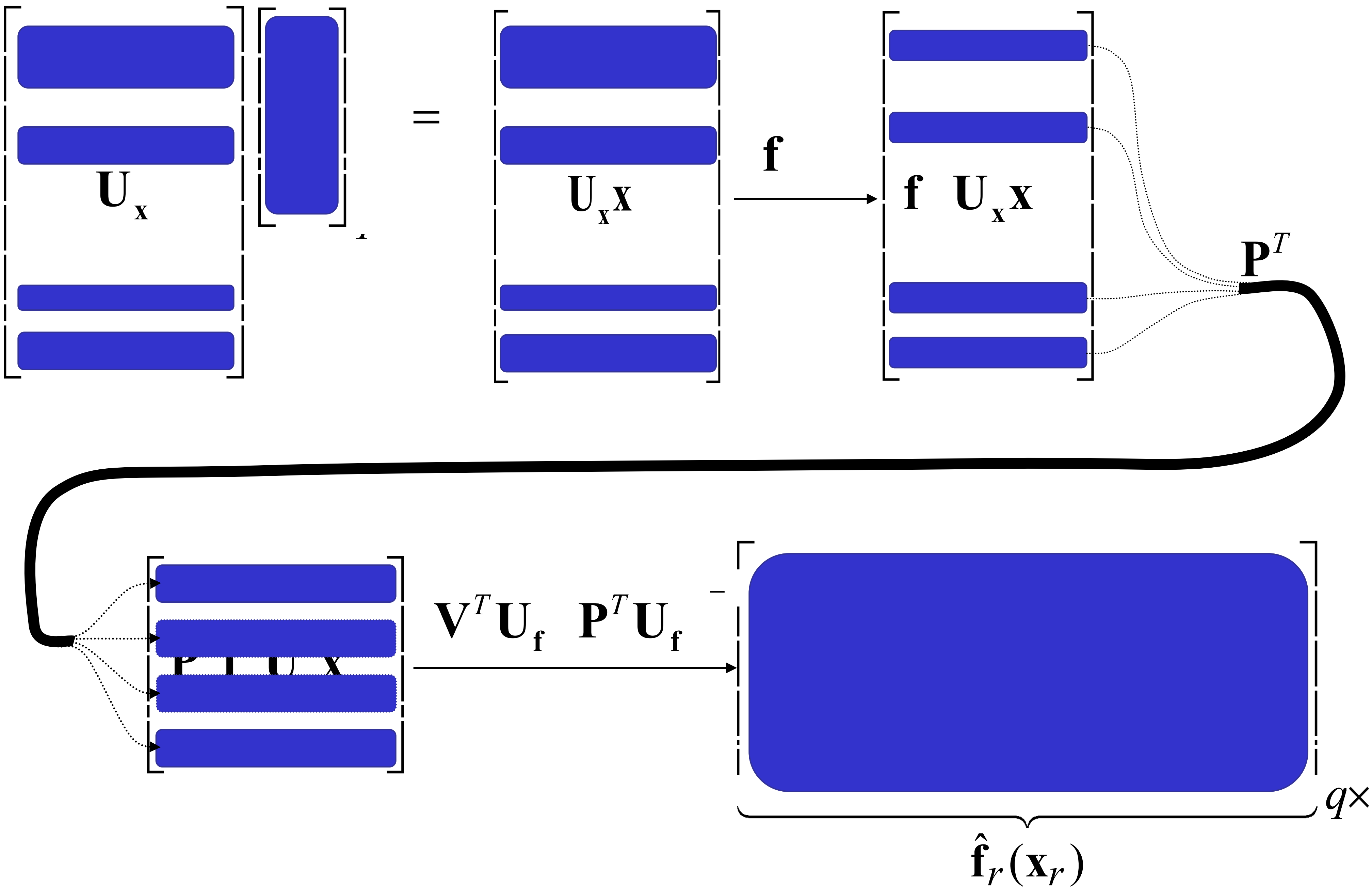
- Where P selects:
  - A few rows of U
  - a few elements of f
    - S. Chaturantabut and D. C. Sorensen, several publications
    - **Empirical interpolation method:** M. Barrault *et al.*, *Comp. Rend. Math.*, 2004.
    - **Missing point estimation:** P. Astrid and A. Verhoeven, Int. Symp. MTNS, 2006.

Picture for a 2-D PDE

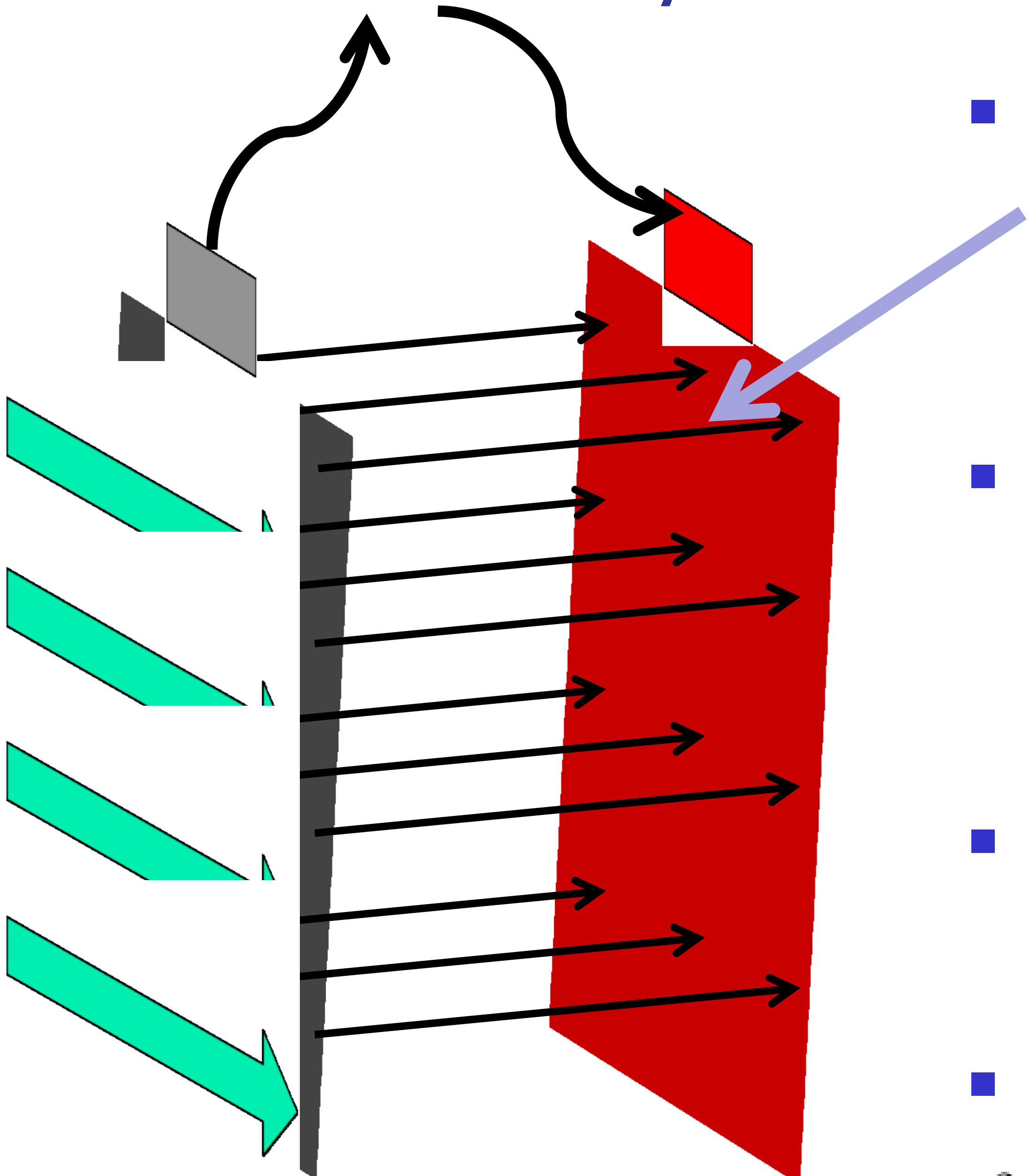


- Evaluate f at approximately q points (black)
- To eval f, need values for x at more points (red)

Discrete Empirical Interpolation Method



Cooled Battery with 1-D Electrochem Model



- NTGK Electrochemistry model

$$i = f(\phi_+ - \phi_-, DOD)$$

$$\frac{d}{dt}DOD = f(\phi_+ - \phi_-, DOD)$$

- Electrical Conductivity Model

$$\sigma_e \nabla^2 \phi_+ = i$$

$$\sigma_e \nabla^2 \phi_- = -i$$

- Thermal Conductivity Model

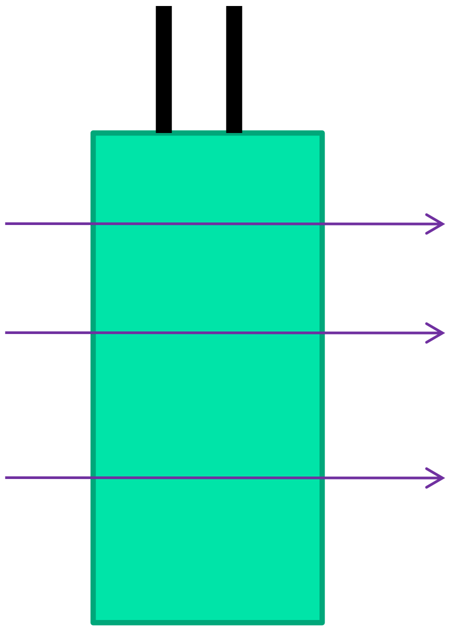
$$\sigma \nabla^2 T = (\phi_+ - \phi_-) * i$$

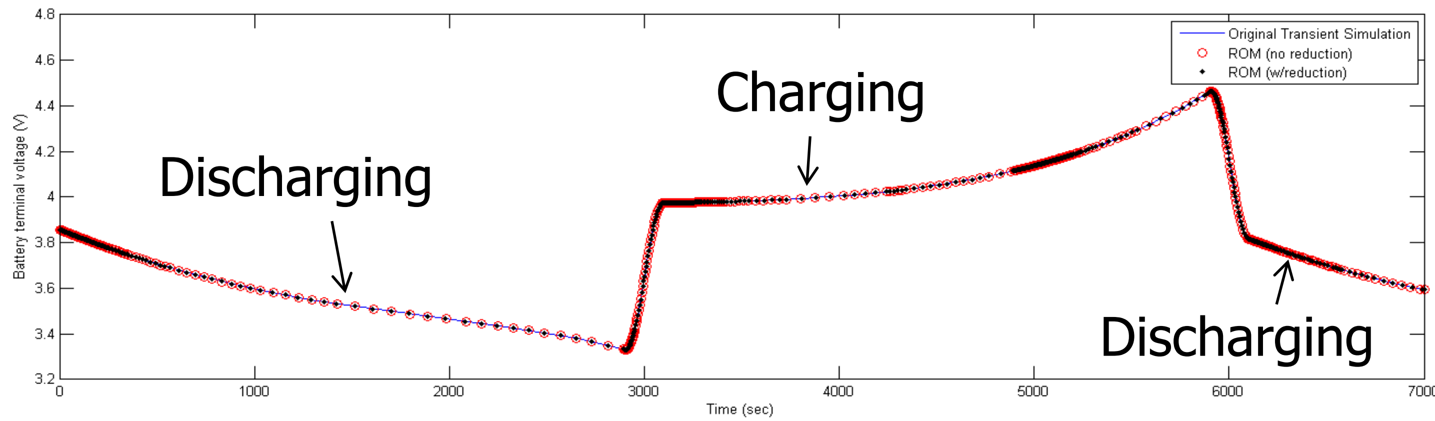
- Sheet Flow Model

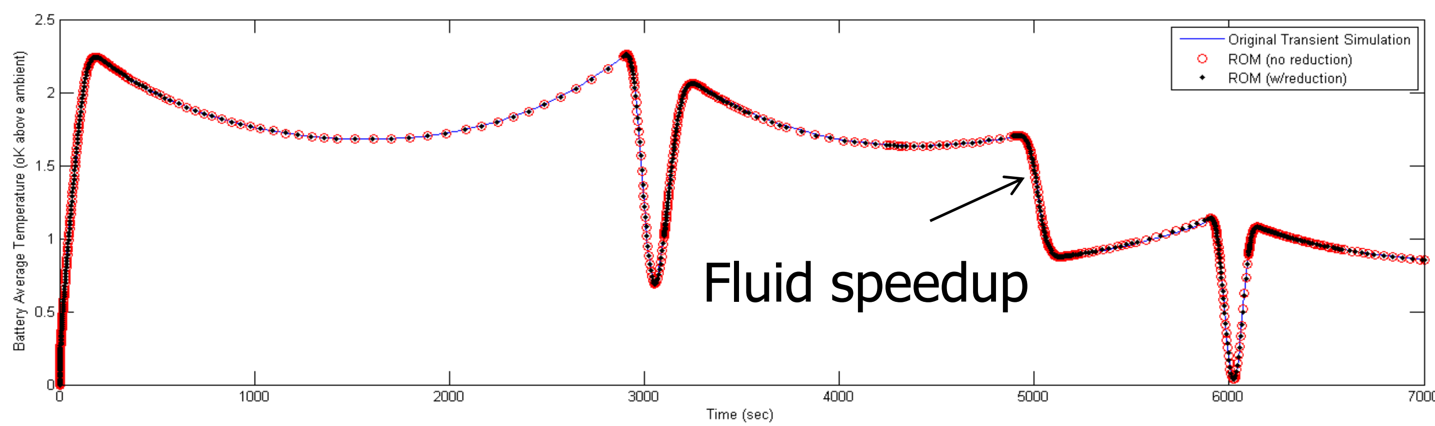
$$\sigma_s \nabla^2 T_s + MFR \cdot \nabla T_s = \alpha \cdot (T_s - T)$$

Transient Results for Fluid Cooled Battery

- Inputs are terminal currents and mass flow rate
- Output is average temperature of fluid out







A New Technique for Every New Technology

- Job security for my students….
- Does Not Scale?
  - Powerful Scripting languages reducing barrier for new techniques.
  - But new “blocks” are not emerging
    - Generalized Fast Solver Software
    - Generic FEM
  - Maybe the issue is interfacing.