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Exact Time-Dependent Kohn-Sham Potential for an Interacting Few-Body System

Rudolph J. Magyar

Shock Physics - 01443
Sandia National Laboratories
Albuquerque, NM 87185

E-mail: rjmagya@sandia.gov

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Materials Problems that Involve Time-Dependent Quantum Mechanical Phenomena

- Secondary electron emission
- Low energy electron-phonon energy transport
- Scattering cross-sections
- Quantum-based molecular dynamics
- Optical transitions

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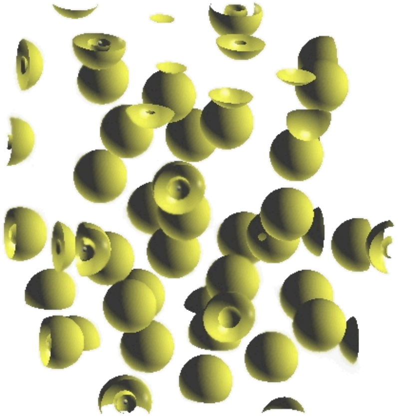
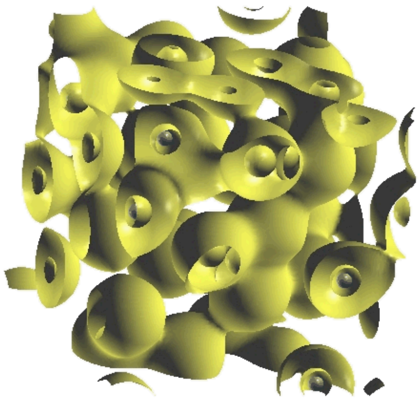




Time-Dependent Density Functional Theory (TDDFT)

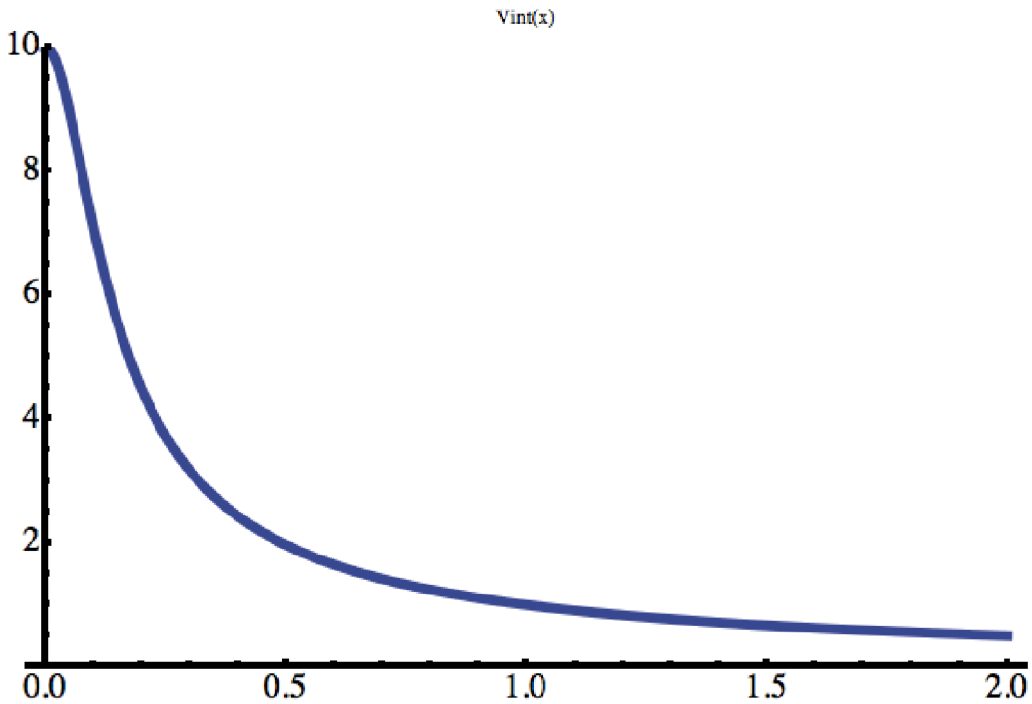
- Quantum electron and nuclear dynamics including many-body physics
- Exact in principle
- Description of electronic excited-states, optical, mechanical, and electronic response properties
- Strength of well developed ground-state theory
- Favorable cost scaling compared to other schemes
- Now available in many common codes for finite systems
- General tools for periodic solids are being developed

Key approximation: $v_{xc}(t)$, the time dependent exchange-correlation potential

We do not know $v_{xc}(t)$ exactly for generic systems!

1D Physics as a Training Set for Approximate Functionals

- Exact many-body results can be found
- Reduced complexity
- Easier to conceptualize
- Model of quasi-1D systems



$$v_{\text{int}}(x) = \lambda / \sqrt{\varepsilon^2 + x^2}$$

- Effective range ε
- Effective strength λ
- Quasi 1D interaction
- No UV divergence

A Many-Body System with Known Time-Dependence

$$H(t)=\begin{cases} -\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2+\sum_{j=1,k=1}^{N,N}v_{\text{int}}\left(x_j-x_k\right)+\frac{\omega}{2}\sum_{j=1}^{N}x_j{}^2, & t<0 \\ -\frac{1}{2}\sum_{j=1}^{N}\nabla_j^2+\sum_{j=1,k=1}^{N,N}v_{\text{int}}\left(x_j-x_k\right)+\frac{\omega}{2}\sum_{j=1}^{N}x_j{}^2+\kappa\sum_{j=1}^{N}x_j, & t\geq 0 \end{cases}$$

$$x_{CM}(t)=x_0+\left(x_i-x_0\right)\cos(\omega t)$$

$$n(x,t)=n_0\left(x-x_{CM}(t)\right)$$

J.F. Dobson, PRL 73, 2244 (1994)

- Natural basis in terms of harmonic oscillator solutions (gaussians, Hermite polynomials)
- Exactly solvable in non-interacting case
- Related to Hookes atom
- Exactly numerically solvable in a basis for few particles
- Suddenly apply a uniform electric field at t=0

Finding the Exact Solution

- Construct entire many particle Hilbert space within a finite basis.
- Diagonalize ground-state.
- Time propagate the solution.
- Restrict ourselves to the more difficult triplet state.

Single Particle Basis

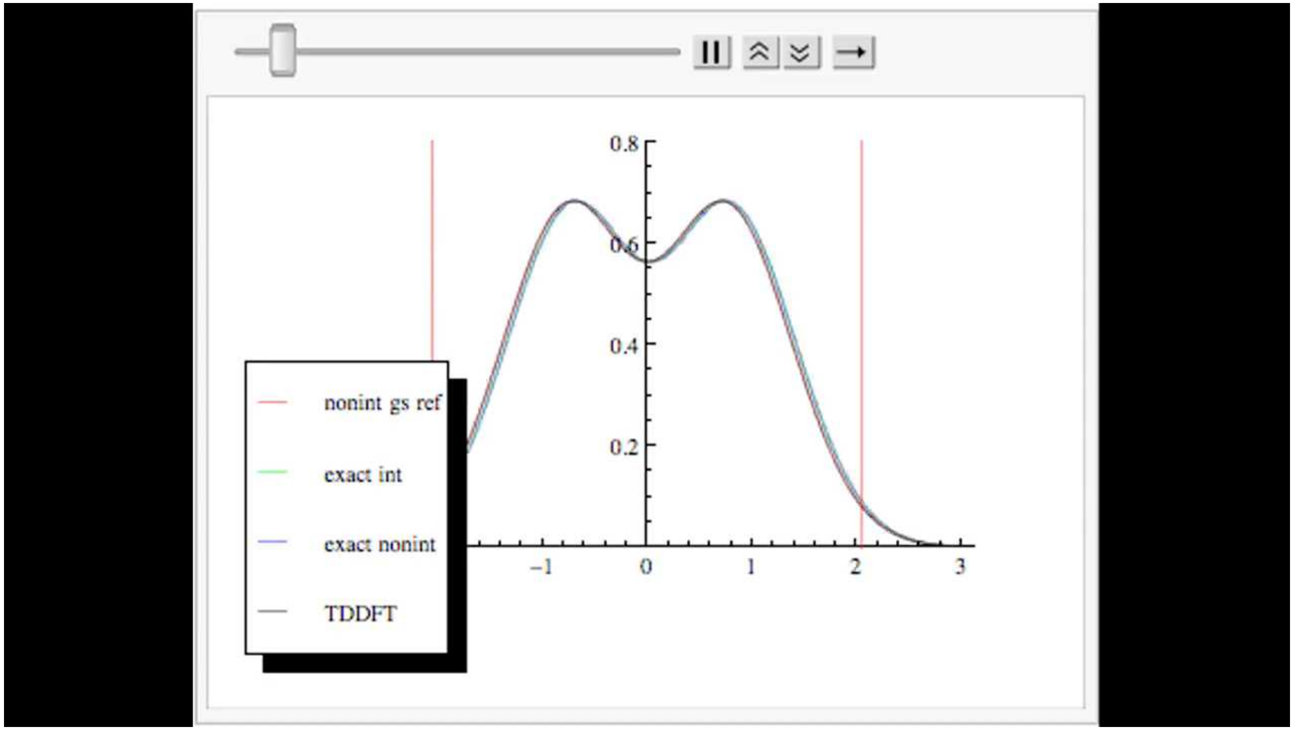
$$|\psi_0\rangle$$
$$|\psi_1\rangle$$
$$|\psi_2\rangle$$

Complete Two Particle Hilbert Space Within Basis

$$\frac{1}{\sqrt{2}}\left(|\psi_0\rangle|\psi_1\rangle - |\psi_1\rangle|\psi_0\rangle\right)$$
$$\frac{1}{\sqrt{2}}\left(|\psi_0\rangle|\psi_2\rangle - |\psi_2\rangle|\psi_0\rangle\right)$$
$$\frac{1}{\sqrt{2}}\left(|\psi_1\rangle|\psi_2\rangle - |\psi_1\rangle|\psi_0\rangle\right)$$

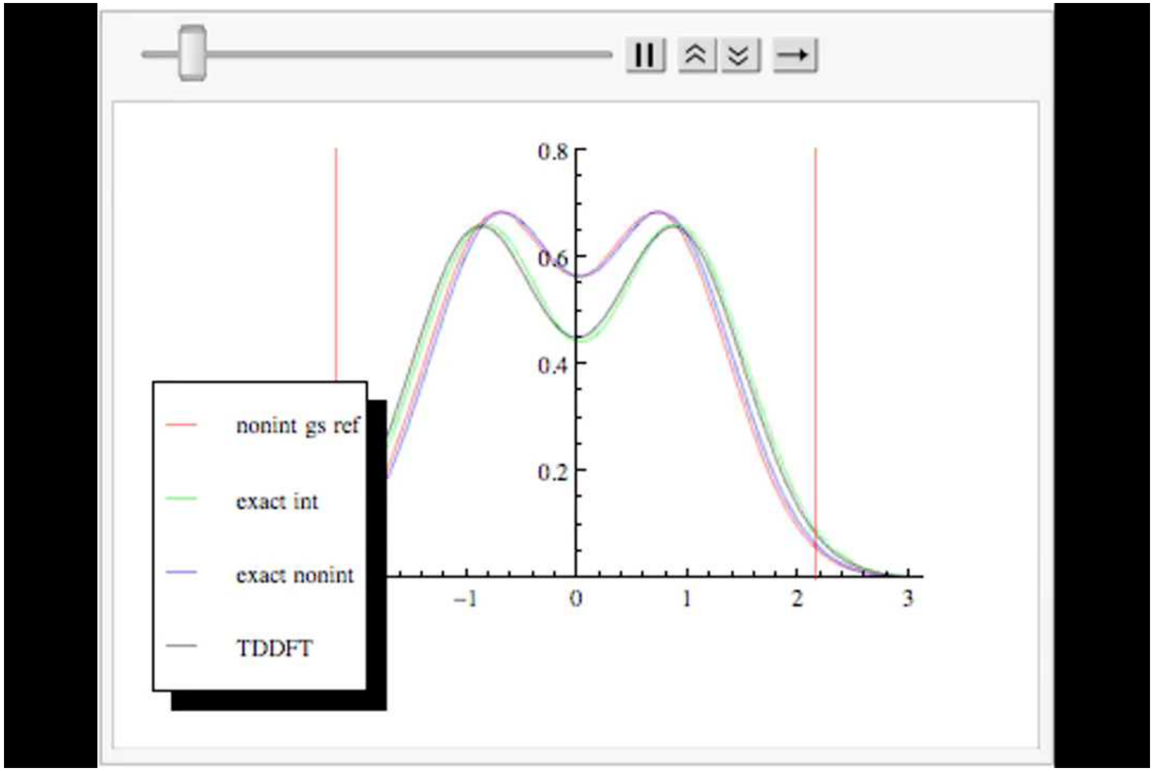
Non-Interacting Time-Evolution for 2 Particles

- Density bounces back and forth as expected!
- Expressed in terms of ground-state harmonic oscillator solutions around x=0
- Spin triplet

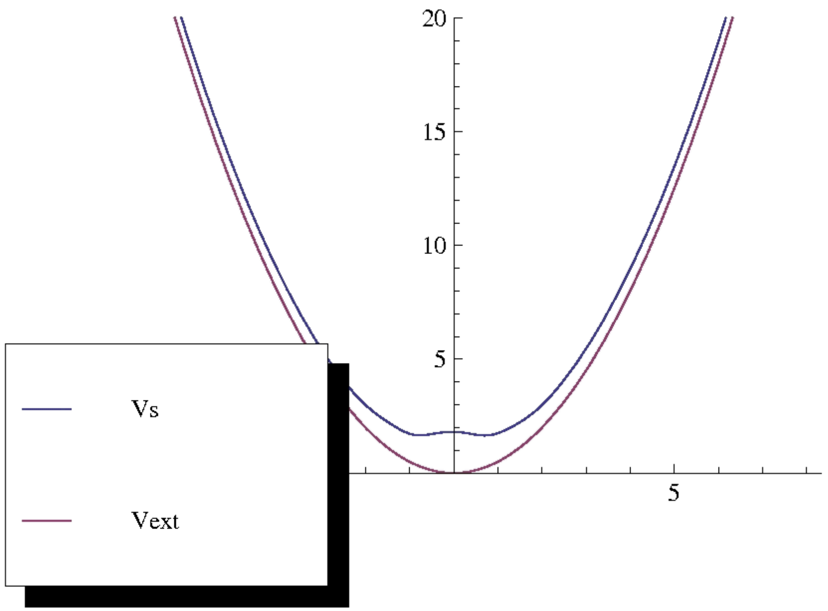


Interacting Time-Evolution for 2 Particles

- Density bounces back and forth as expected.
- Note that the interacting density is expanded relative to the non-interacting one.
- In the finite basis complete Hilbert space, no special changes are needed to the time integrator.



Extracting the Exact TD-KS Potential



- For Ground-state: Van Leeuweens: Iterative scheme to find v_{ks} using the density as the target.
- W. Yang's: Iterative scheme to find v_{ks} using the Hartree potential as the target.
- For time dependence, this has never been done for more than two particles in a singlet beyond the adiabatic limit.
- Method must be generally applicable to be useful, not restricted to this model.

Method to Obtain V_{ks}

$$n(r,t) = \sum_{i}^{occ.} \left|\phi_i(r,t)\right|^2$$

$$i\frac{\partial}{\partial t}\phi_i(r,t) = \left[-\tfrac{1}{2}\nabla^2 + v_{KS}\left[\Psi_0,\Phi_0,n\right](r,t)\right]\phi_i(r,t)$$

$$\delta n(y,t_1) = \chi_{KS}(y,x,\Delta t)\,\delta v_s(x,t_0)$$

- $n_1(x)$ is the target density
- $\phi_{-1}(x)$ are assumed known
- Δ is the time step
- $v_s(x,t)$ is the average potential between start and end times over the interval
- Iterative scheme

$$\begin{pmatrix} \phi_{-1} \\ n_{-1} \\ \\ \end{pmatrix} \xrightarrow{\Delta/2} \begin{pmatrix} \\ \\ v_{s,0} \end{pmatrix} \xrightarrow{\Delta/2} \begin{pmatrix} \phi_1 \\ n_1 \\ \\ \end{pmatrix}$$

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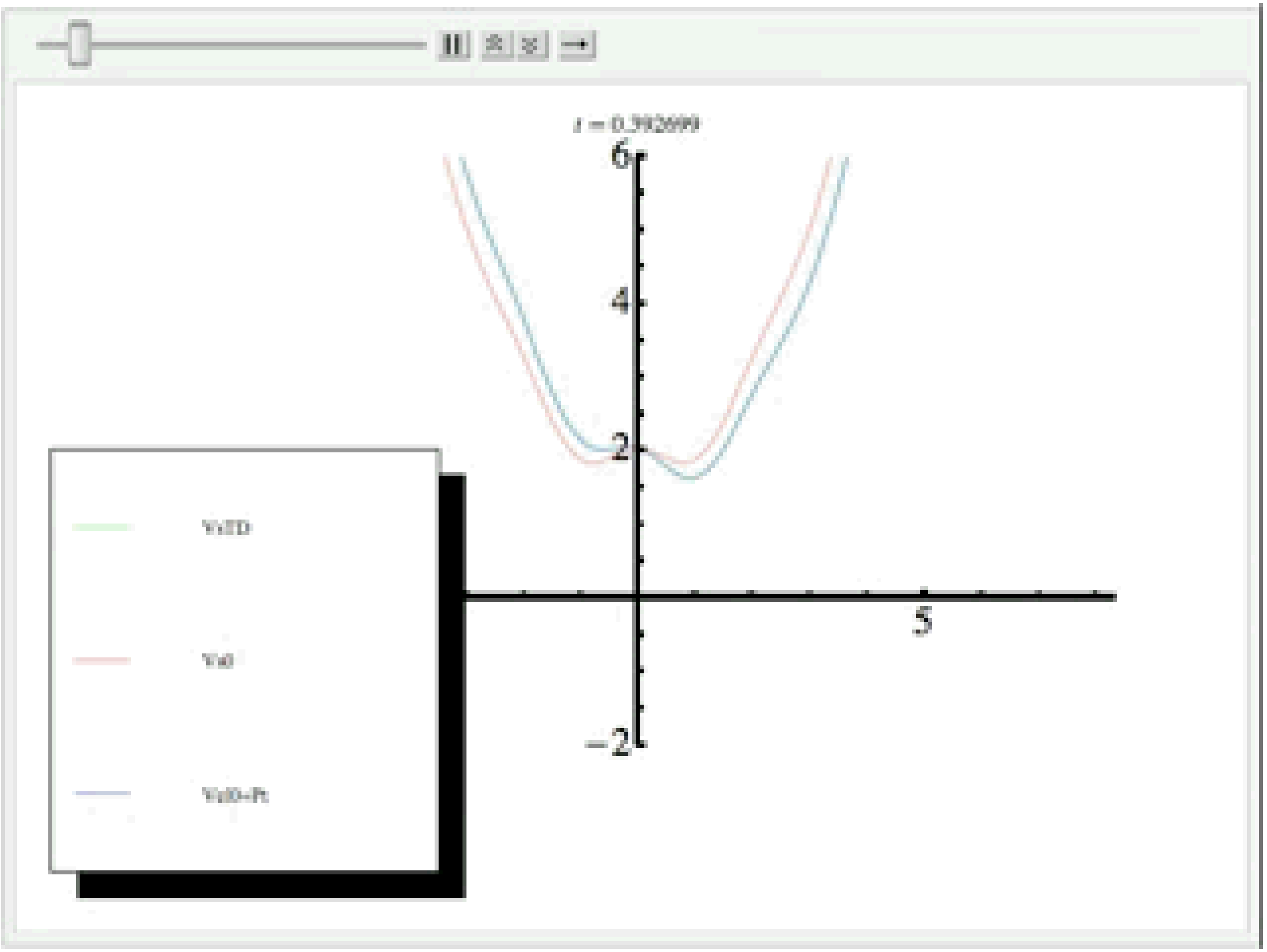
V_{ks} TD Exact

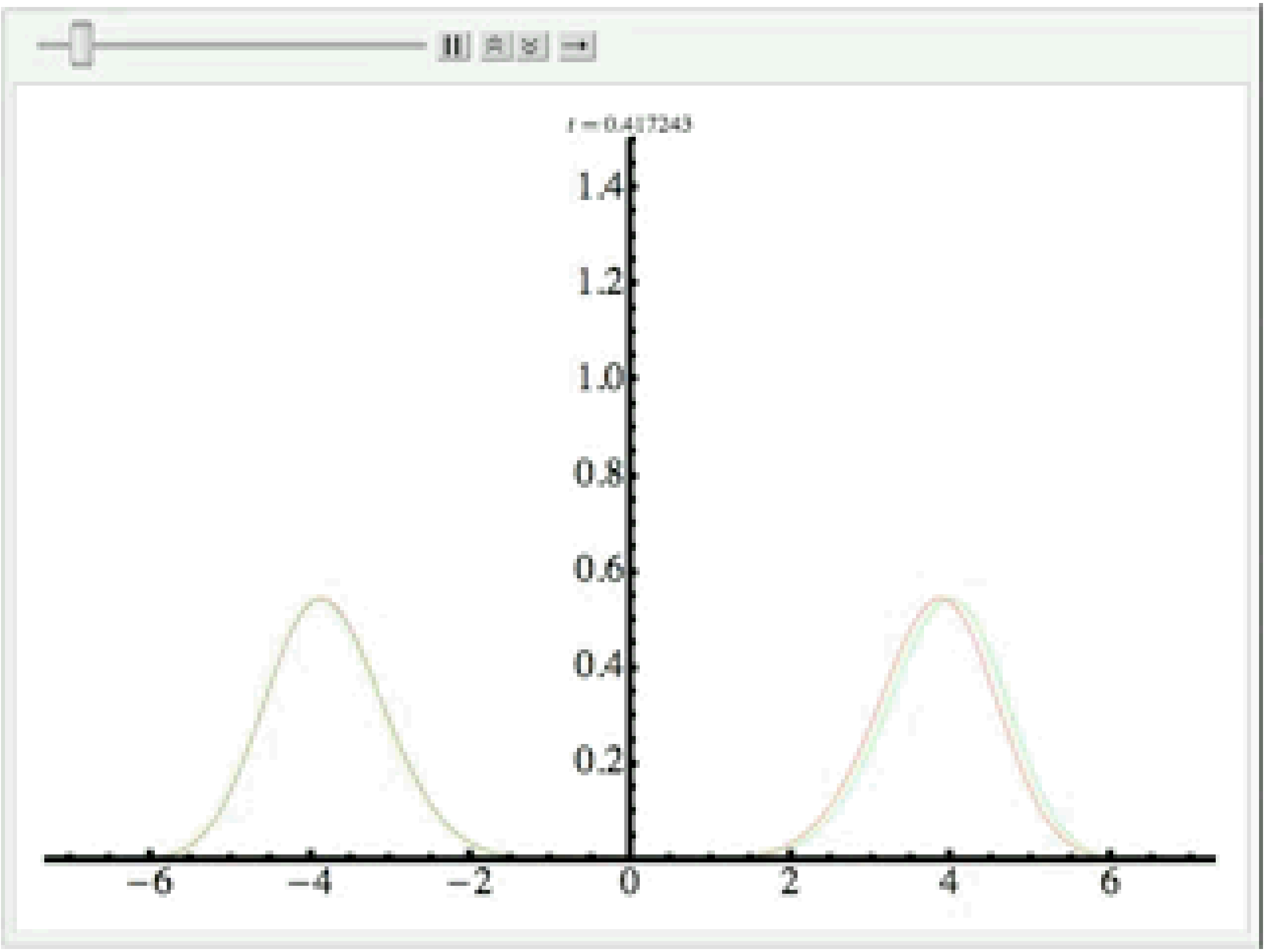


Conclusions and Thanks

- Kohn-mode oscillations offer one of the few exactly solvable time-dependent many electron systems with an analytically known density evolution.
- There is still more to be learned for use in TDDFT by studying harmonically trapped electrons.
- In particular, this system offers a testing ground for time-integrators, basis set limitation questions, and fundamental issues regarding adiabatic and local exchange-correlation potential functionals.

- **Thanks to ….**
- **Audience**
- **APS**
- **LDRD - Low Energy Electron-Photon Transport**
- **Harry Hjalmarson, Ann Mattsson, Luke Shulenberger, Peter Shultz**

Double Well – Potential to Study Discontinuity



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