

# Stochastic Electrodynamic Simulation of Hydrogen Ground State

D. Reitz

# Background

# Stochastic Electrodynamics

- Stochastic Electrodynamics (SED)
- Classical theory with electromagnetic background radiation
- Lorentz-Invariant radiation field similar to Zero-Point Field of Quantum Electro Dynamics (QED)
- Attempts to provide physical description for quantum and probabilistic observations

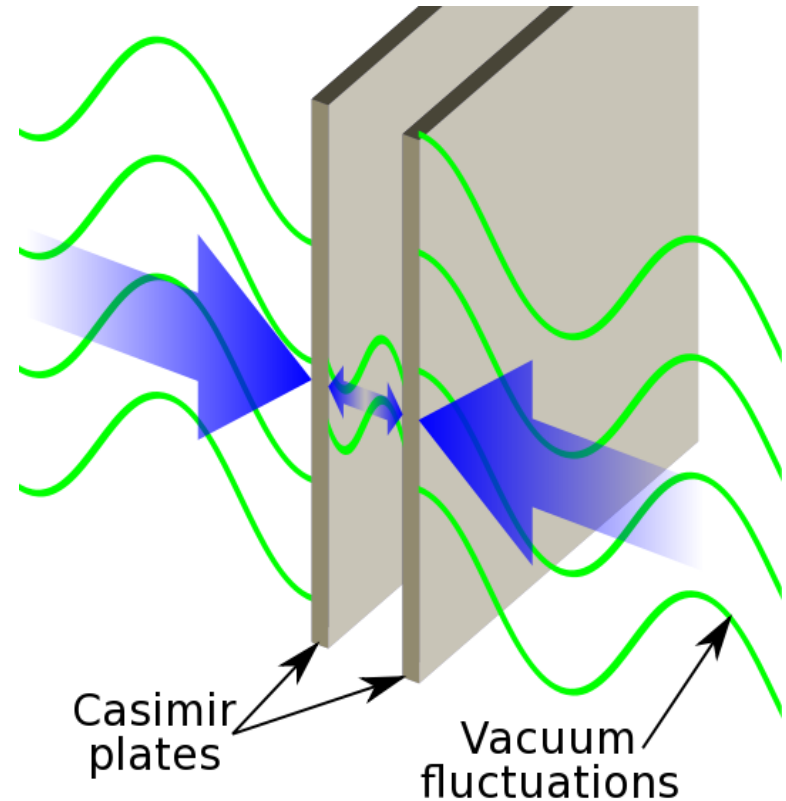
# History

- Marshall and Boyer in 60's and 70's with some times to earlier works of Nerst, Einstein, and Planck
- Casimir Force
- Van der Waals Force
- Diamagnetism

Ref: [1] and Wikipedia

# Illustration

- Casimir Force concept  
illustration of the  
background field of SED



[http://en.wikipedia.org/wiki/File:Casimir\\_plates.svg](http://en.wikipedia.org/wiki/File:Casimir_plates.svg)

# Other Areas

- Pioneer / Controversial
  - Harmonic Oscillator
  - Ground State of Hydrogen Atom
- More Speculative State
  - de Broile waves
  - Inertia
  - Gravitation

Ref: [1] and Wikipedia

# H Ground State Simulation

- Late 70's – 80's inconsistency with non-linear systems.
- Interest dwindled
- Proposals that non-linear systems are inadequate for describing atomic/molecular systems
- Coulombic binding potential proposed as necessary for accurate description
- Analytical solutions difficult
- Thus simulation steps in

# SED Simulation

Pictures and equations From D. C. Cole, *Simulation results related to stochastic electrodynamics*

- D. C. Cole, "[Simulation results related to stochastic electrodynamics](#)," published in AIP Conference Proceedings Vol. 810, No. 1, pp. 99-113. The international conference was entitled "Quantum Theory: Reconsideration of Foundations-3," and was held June 6-11, 2005, at Växjö University, Sweden. Proceedings edited by G. Adenier, A. Khrennikov, and T. Nieuwenhuizen.
- Non-windowing simulation from that paper is the basis for project
- Paper and graphics from Cole used throughout report and following slides

# The Math

- Background Radiation Field Spectrum

$$\rho(\omega) = \frac{\hbar\omega^3}{2\pi^2c^3} = \frac{\omega^2}{\pi^2c^3} \frac{\hbar\omega}{2}$$

- Relativistic Lorentz-Dirac EOM

$$m \frac{d^2 z^\mu}{d\tau^2} = \frac{2q^2}{3c^3} \left[ \frac{d^3 z^\mu}{d\tau^3} - \frac{1}{c^2} \left( \frac{d^2 z^\lambda}{d\tau^3} \frac{d^2 z_\lambda}{d\tau^3} \right) \frac{dz^\mu}{d\tau} \right] + F^\mu$$

- $z^\mu$  is the four vector space-time position
- $m$  is the particle normalized mass
- $q$  is the charge
- $\tau$  is the particle proper time
- $F^\mu$  is the sum of all four-vector forces acting on the particle

(this is typically the binding potential, the Lorentz force due to radiation fields, and other applicable external forces)

# More Math

- Radiation Field Sum of Plane Waves

$$\mathbf{E}(\mathbf{x}, t) = \sum_{n_x, n_y, n_z = -\infty}^{\infty} \sum_{\lambda=1,2} \frac{\hat{\mathbf{e}}_{\mathbf{k}_n, \lambda}}{(L_x L_y L_z)^{1/2}} [A_{\mathbf{k}_n, \lambda} \cos(\mathbf{k}_n \cdot \mathbf{x} - \omega_n t) + B_{\mathbf{k}_n, \lambda} \sin(\mathbf{k}_n \cdot \mathbf{x} - \omega_n t)]$$

- With periodic boundary conditions:

$$\mathbf{k}_n = \frac{2\pi n_x}{L_x} \hat{\mathbf{x}} + \frac{2\pi n_y}{L_y} \hat{\mathbf{y}} + \frac{2\pi n_z}{L_z} \hat{\mathbf{z}}$$

where  $n_x$ ,  $n_y$ , and  $n_z$  are integers,  $\omega_n = c|\mathbf{k}_n|$ ,  $\mathbf{k}_n \cdot \hat{\mathbf{e}}_{\mathbf{k}_n, \lambda} = 0$ , and  $\hat{\mathbf{e}}_{\mathbf{k}_n, \lambda} \cdot \hat{\mathbf{e}}_{\mathbf{k}_n, \lambda'} = 0$  for  $\lambda \neq \lambda'$ .

- A and B are a Gaussian distribution that correlate by frequency and Temp as follows

# More Math

- Spectral Energy Density Correlation

$$\rho(\omega, T) = \frac{\omega^2}{\pi^2 c^3} \frac{f(\omega, T)}{4\pi}$$

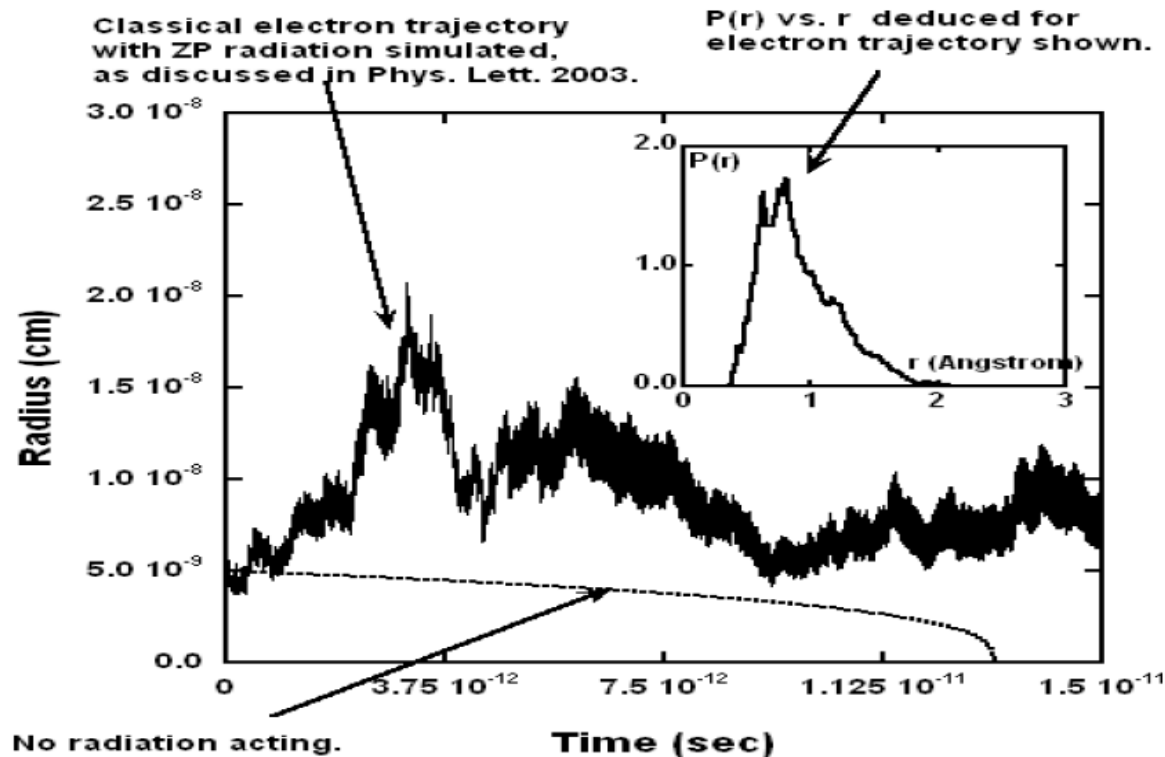
with  $f(\omega, T) \rightarrow 2\pi\hbar\omega$  as  $T \rightarrow 0$ .

- The Coulombic binding potential (nucleus to electron)

$$m \frac{d^2 \mathbf{z}}{dt^2} = -\frac{e^2 \mathbf{z}}{|\mathbf{z}|^3} + \frac{2 e^2}{3 c^3} \frac{d^3 \mathbf{z}}{dt^3} + (-e) \left\{ \mathbf{E}[\mathbf{z}(t), t] + \frac{\dot{\mathbf{z}}}{c} \times \mathbf{B}[\mathbf{z}(t), t] \right\}$$

# SED Simulation Illustration

- Classically without ZP radiation electron goes to  $r=0$  within  $1.3e-11$  s



# Why?

- SED has appeal in that introduces an explanation for some observations
- 2005 Paper indicated days (i.e. 900) computer time
  - Applying concepts from the course would benefit the simulation
- Goal
  - Increase knowledge of SED simulation
  - Improve the computational performance of the numerical simulation
  - Potential future rigorous evaluation / development of SED model of H ground state

# Serial Approach

# Serial Approach

- The author of [1] was contacted to request simulation code of non-windowing approach
- Initial results
  - Over 26 to 48+ hours to execute to  $2.0e-10$  s
  - Results invalid on gmice
- Spend a bunch of time trying to eliminate precision issues
  - Unstable results take hours to get to
  - Went down path of long doubles and functions throughout
    - Negative impact on run times

# Serial Approach

- Eventually back on track with sticking with doubles and careful tweaking of constants and initial conditions
- Focus on limiting simulation runs to  $1.6e-11$  seconds

# Serial Approach

- Code Overview
  - Allocate and initialize global storage and constants
  - Initialize random plane waves
  - Solve using 5<sup>th</sup> Order Runge-Kutta with adaptive step size
    - until done
      - rkqs -> rkck -> computes loops -> calls derivs (5 times each pass)
      - derivs is the radiation field sum of plane waves

# Optimization

- Optimizations benefiting serial and parallel
- Analysis
  - Derivs is called many, many times - look at ways to optimize that functional
  - Eliminate repeated allocation and deallocation of memory where possible
  - Reuse computed information where possible

# Optimization Examples

- In Derivs

```
for (i=Nmin; i<=Nmax; i++)
{
    // dreitz - optimize
    // Ex=sqrt(i)*(Amplitude1[i]*cos(theta)-Amplitude2[i]*sin(theta))+Ex;
    // Ey=sqrt(i)*(Amplitude3[i]*cos(theta)-Amplitude4[i]*sin(theta))+Ey;
    const long double& theta=omega*i*x;
    const long double& s=sin(theta);
    const long double& c=cos(theta);
    const long double& sqrt_i=sqrt(i);
    Ex += sqrt_i*(Amplitude1[i]*c - Amplitude2[i]*s);
    Ey += sqrt_i*(Amplitude3[i]*c - Amplitude4[i]*s);
}
```

- Replaced allocate & delete of memory where possible in functions

# Parallel Approach

# Parallel Approach

- Parallelizing a 5<sup>th</sup> order Runge Kutta method is a challenge
  - Not a trivial parallelization task
- Analyzed function calls and flow to identify candidate parallel sections
- For loops in rkck are only loops of 4 with a single line of calculations
  - Cost of parallelization (sync or comm) exceeds expected benefit

# Parallel Approach

- Derivs() loops identified as candidates for parallelization
  - Loops regularly of 10000+
  - This function is called repeatedly
  - OpenMP selected as a good candidate
    - Ease of parallelizing loop
    - Quick and easy syntax for reduction and synchronization
  - MPI not pursued
  - Scalable across SMP computational platforms
  - MPI candidate for this section if larger plane wave sets

# Parallel Approach

- Static to minimize synchronization overhead
  - Work per thread fixed so can be pre-determined
  - In some runs `schedule(dynamic, 1536)` was used
  - 8 effective Core Xeon Nehalem system used (8 threads)
- Summary of OpenMP parallelization

```
#pragma omp parallel for schedule(static) reduction(+:Ex) reduction(+:Ey)
for (i=Nmin; i<=Nmax; i++)
{
    const double& theta=omega*i*x;
    const double& s=sin(theta);
    const double& c=cos(theta);
    const double& sqrt_i=sqrt(i);
    Ex += sqrt_i*(Amplitude1[i]*c - Amplitude2[i]*s);
    Ey += sqrt_i*(Amplitude3[i]*c - Amplitude4[i]*s);
}
```

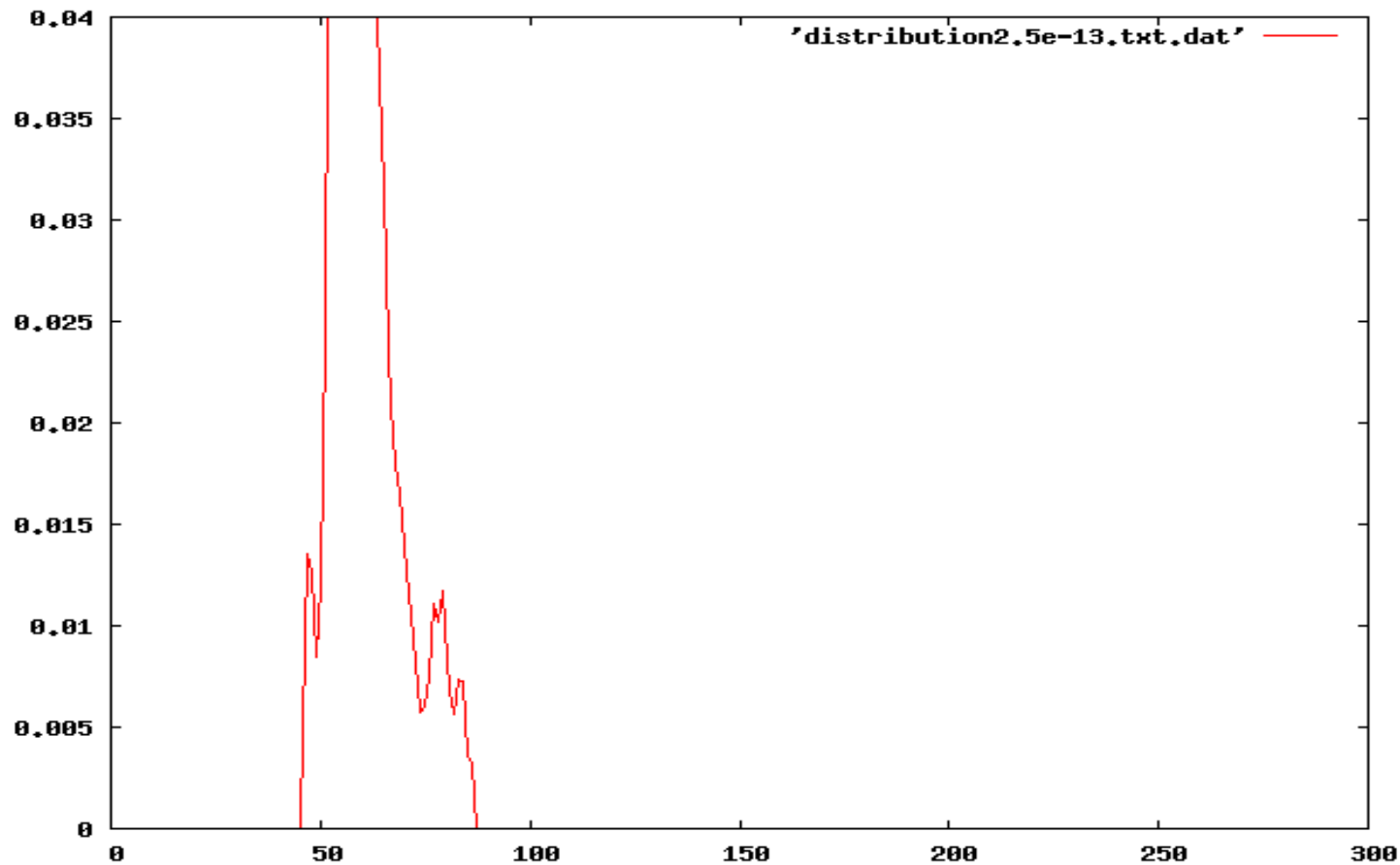
# Performance Comparison

# Results

- Parallel Version 10.6 hours (8 core/threads)  $t$  to  $1.6e-11$

– Animated results:

<http://www.csi702.net/csi702/index.php/Image:Hsed-animate.gif>



# Performance Comparison

- Gmice issue and latter time unavailability
- Initial serial run was 26-48+ hours ( $t=2.0e-10$ )
- Estimated serial run in final config (still running)
  - 16h based on earlier runs
- Difficult to compare results
  - Distribution sensitive to any change in precision
    - parallel math sequence differences can yield different distributions
    - Distributions at smaller  $r$  dramatically increase compute time

# Lessons Learned

# Lessons Learned

- With codes that take a lot of time to run
  - Start early
  - Understand code
  - Avoid brute-force solutions to issues
  - Patience
  - Access to computing resources important
    - The more the better to evaluate permutations
  - Keep record and track of permutations

# Recommendations

- SED Simulation of Hydrogen Ground State
  - Still much to do
  - Precision stability needs further analyzed, understood, and eliminated or reduced
  - Useful for further analysis and theory development