Calculating energy levels by solving the generalized eigenvalue problem

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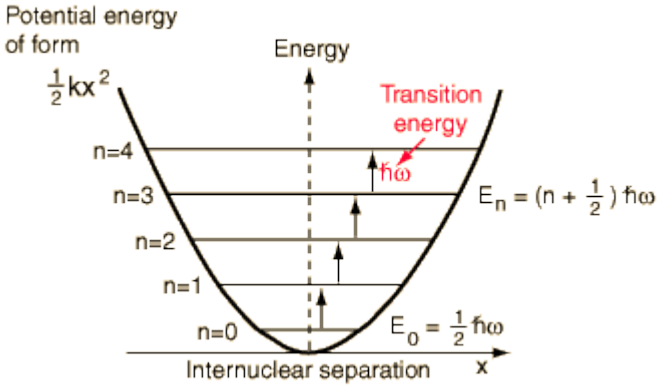
Description and overview

- We use the Monte Carlo method to calculate the lowest energy levels for
  - harmonic oscillator
  - double well potential
    - calculate the tunneling time
- Parallelize simulation



Some Theory

$$C_{ij}(t) \quad = \quad \langle O_i(t) O_j^*(0) \rangle = \sum_{n=1}^{\infty} \mathrm{e}^{-E_n t} \psi_{ni} \psi_{nj}^* \,, \quad i,j = 1, \ldots, N$$

$$\psi_{ni} \equiv (\psi_n)_i = \langle 0 | \hat{O}_i | n \rangle \quad E_n < E_{n+1} \,.$$

Operators need to distinguish between states of interest

The generalized eigenvalue problem

- $$C(t)\, v_n(t, t_0) = \lambda_n(t, t_0)\, C(t_0)\, v_n(t, t_0)$$

$$\lambda_n(t, t_0) \propto e^{-E_n(t-t_0)}\left(1 + o\left(e^{\Delta E(t-t_0)}\right)\right)$$

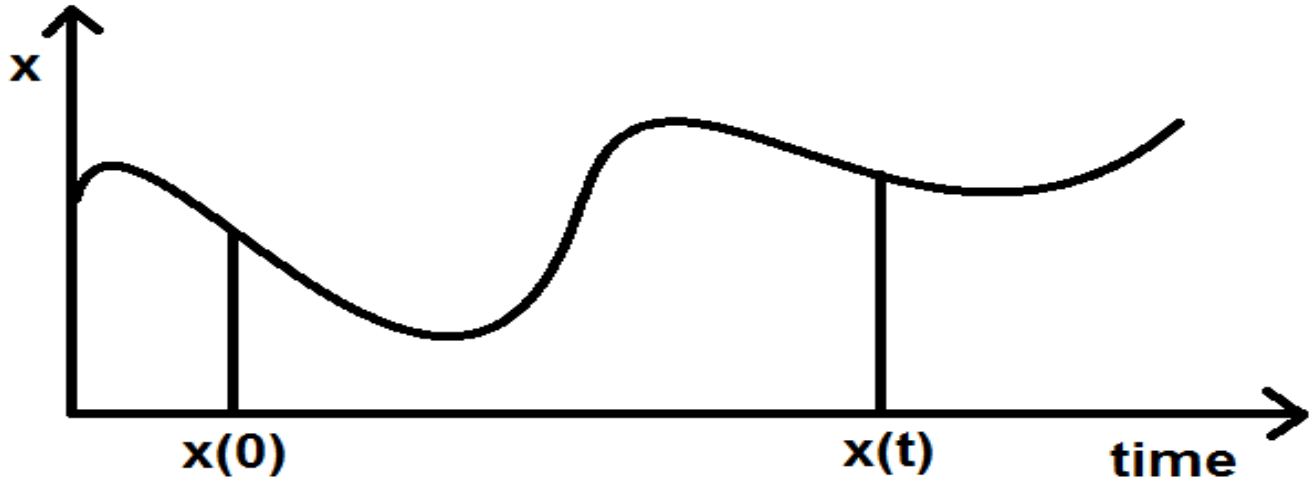
$$\begin{aligned} E_n &= \lim_{t\to\infty} E_n^{\mathrm{eff}}(t, t_0)\,, \\ E_n^{\mathrm{eff}}(t, t_0) &= -\partial_t \log \lambda_n(t, t_0) \equiv -\frac{1}{a}\left[\log \lambda_n(t + a, t_0) - \log \lambda_n(t, t_0)\right] \end{aligned}$$

Accuracy

- As the correlation signal decays exponentially, the noise quickly becomes significant
- But we also need to measure the eigenvalues at a large t to reduce influence from other states

Correlation time for path

$$C_{ij}(t) = \left\langle x^i(0) x^j(t) \right\rangle$$



t = correlation time

Correlation matrix

$$C_{ij}(t) = \left\langle x^i(0) x^j(t) \right\rangle$$

- We use 6 powers to extract 4 energy levels
  - 6x6 matrix
- We calculate this for 15 correlation times and for all N ~ 1000 elements
- And typically 10^5 samples
  - 6^2x15x1e3x1e5 ~ 5e10 operations

Jackknife Errors

- Estimate errors for complex calculations where normal error calculations are not feasible
- Resampling from a set of observations by removing a number of them
- Recompute the result for several smaller sample sizes to estimate the error

$$\sigma^2_{\mathrm{Jmean}} = (N-1)\sum_{i=1}^{N}(m_{Ji} - m)^2/N$$

http://www.physics.utah.edu/~detar/phycs6730/handouts/jackknife/jackknife/jackknife.html

Harmonic Oscillator

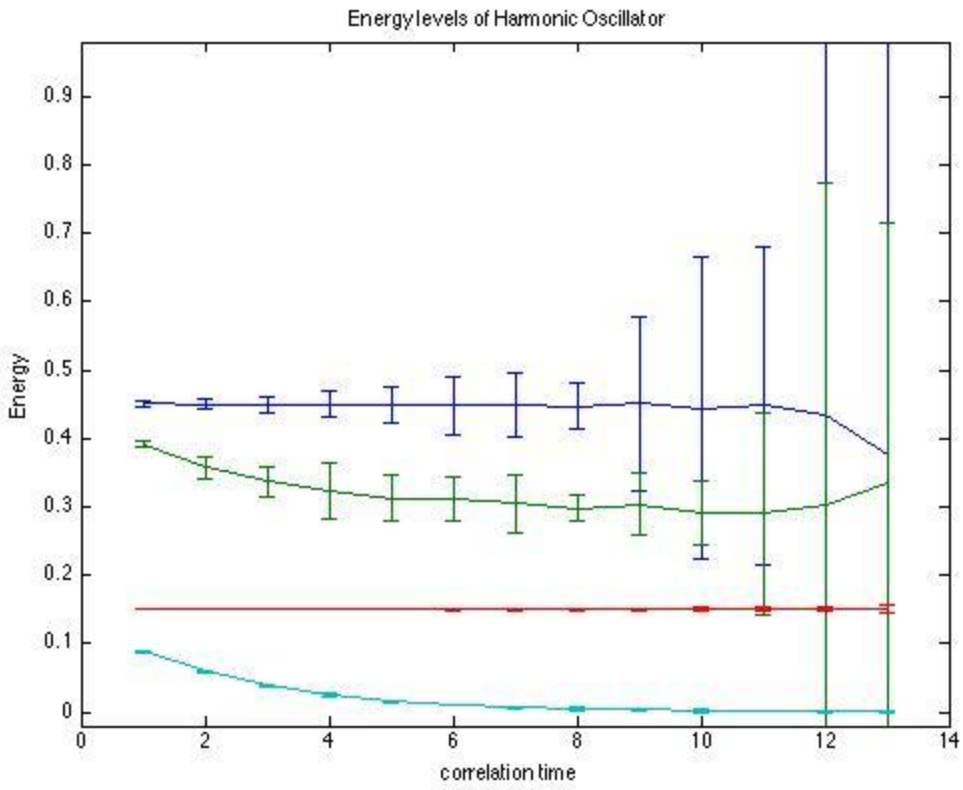
- $\omega = 0.15$
- $a = \varepsilon = 1$
- $m = 1$
- $V(x) = \frac{1}{2}x^2$

- The error bars was calculated by jackknife error estimate

CPU

- N_path = 1e3
- samples = 1e6
- separation = 10
- maxStep = 1
- 338 minutes

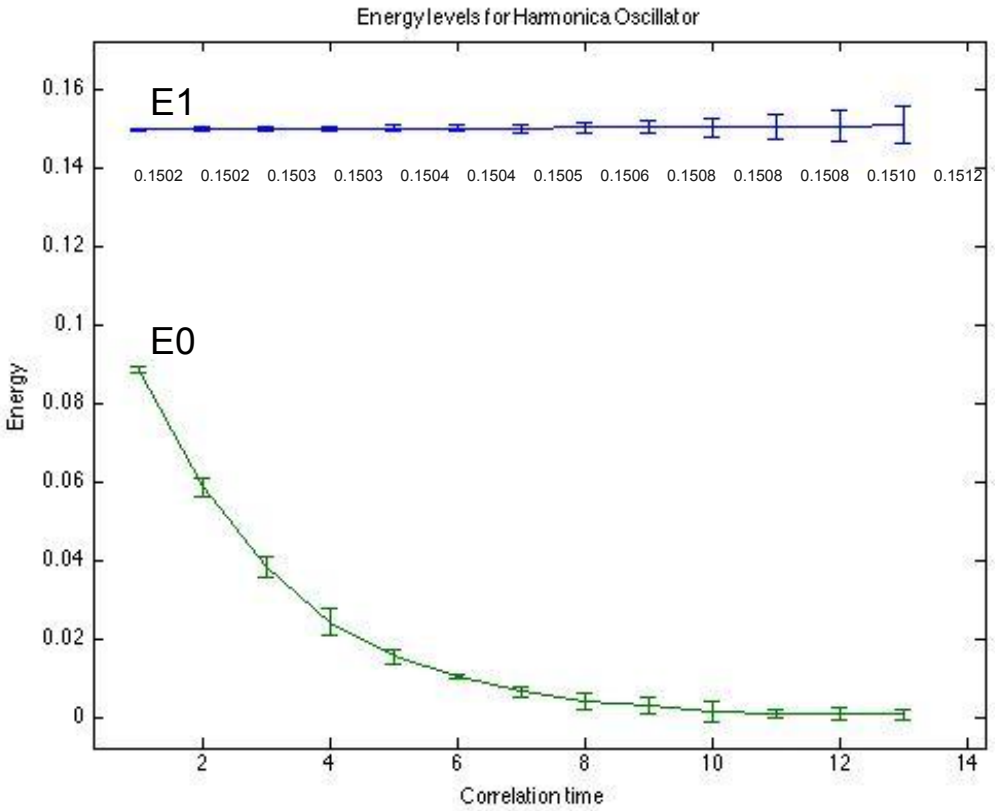
- ω_shift = 0.1504



CPU

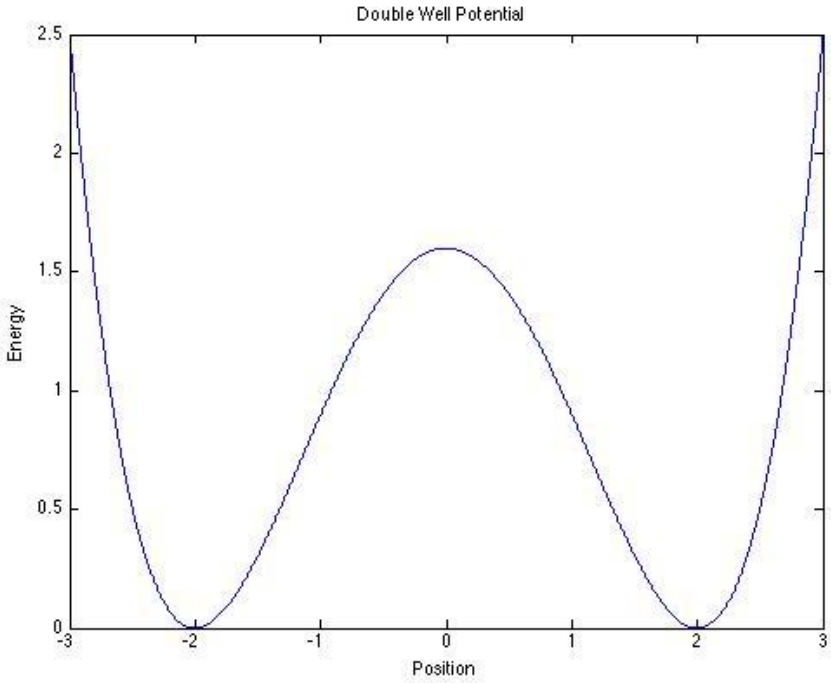
- N_path = 1e3
- samples = 1e6
- separation = 10
- maxStep = 1

- dω = 0.1505
- ω_shift = 0.1504



Double Well

- V(x) = λ(x^2 - v^2)^2
- λ = 0.1
- v = 2
- Barrier height = 1.6

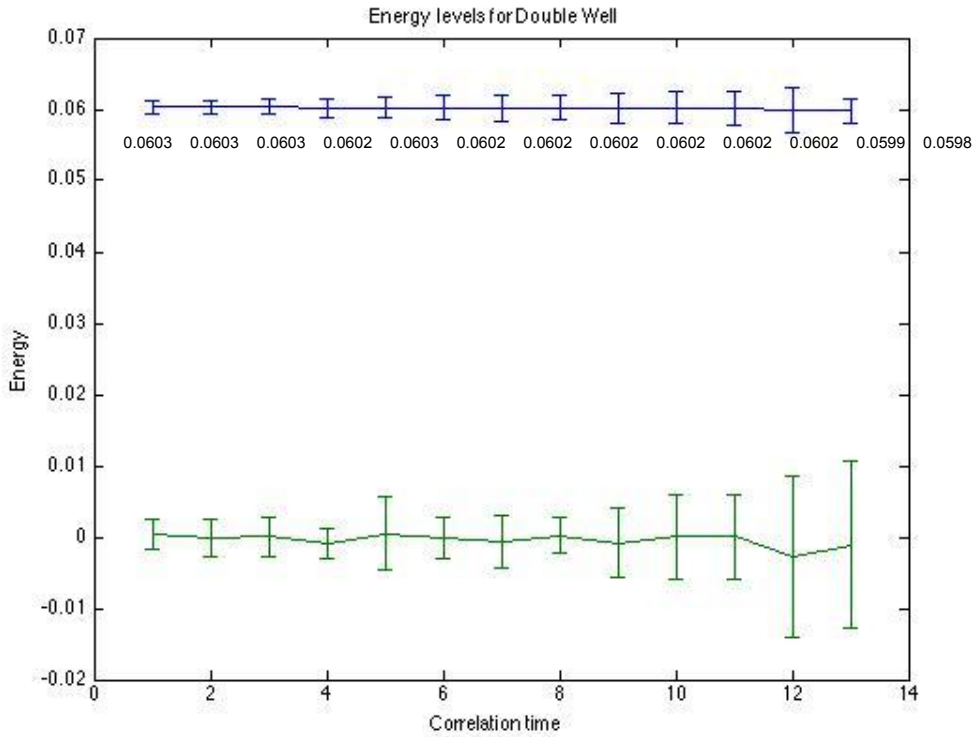


- ω_HO = 1.8
- E0_HO = 0.9

CPU

- N_path = 1e3
- samples = 1e6
- separation = 10
- maxStep = 1
- 341 minutes

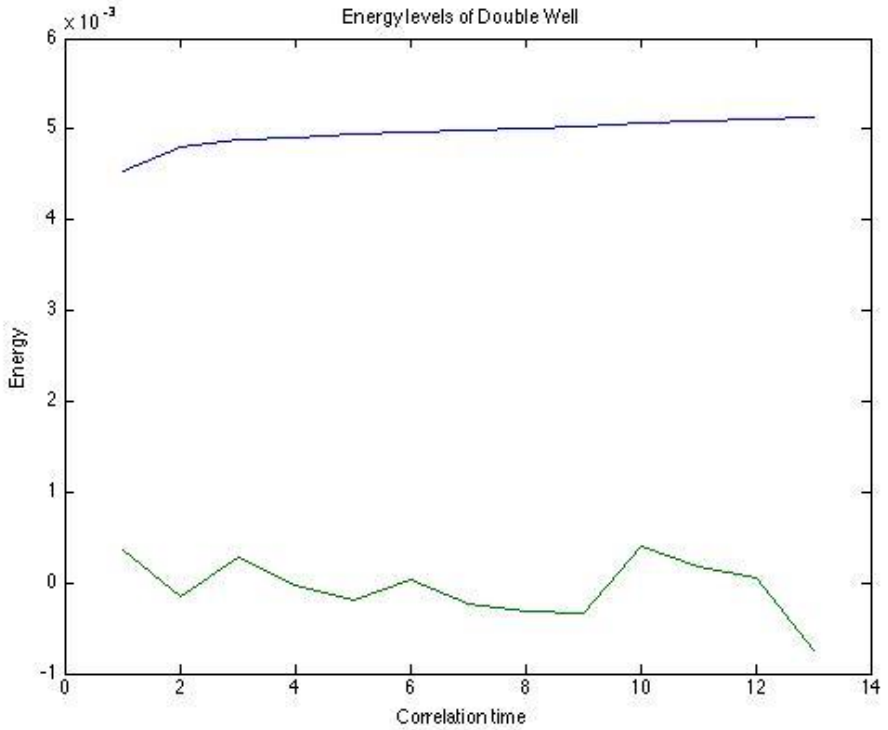
- dω = 0.0602
- t = 1.32
- ω_HO = 1.8



GPU

- samples = 1e5
- λ = 0.23
- v = 2
- Barrier height = 3.68

- ω_HO = 2.7
- dω = 0.00484
- t = 16.6
- Huge errors



CPU vs GPU

- Can we leverage the massively parallel power of the GPU to speed up the computation of the energies?

GTX Titan (8 in the igpu6 machine):

14 Multiprocessors (192 per SMX)

2688 CUDA Cores

2048 Threads max per SMX

Path Generation Benchmarks

- Path generation can be sped up withe the GPU
- Implementation is a bit more invovled however

		10k	100k	1mil
CPU Code	Intel i7	.97 s	9.72 s	98.0 s
GPU Code	GTX 770	0.32 s	2.7 s	26.4 s
	GTX Titan**	13.3 s	13.5 s	48.4 s

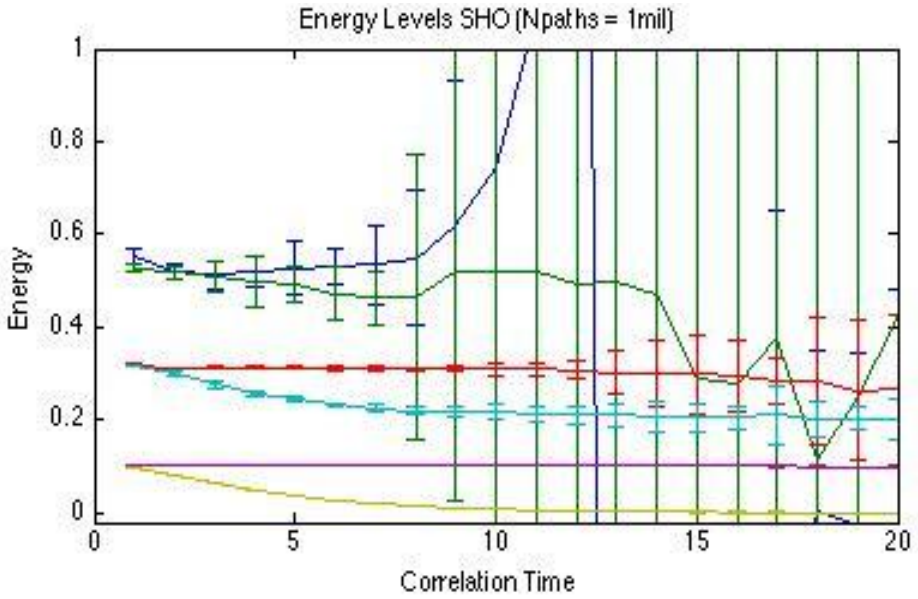
**Noticeably longer start up time for Titan ~10s

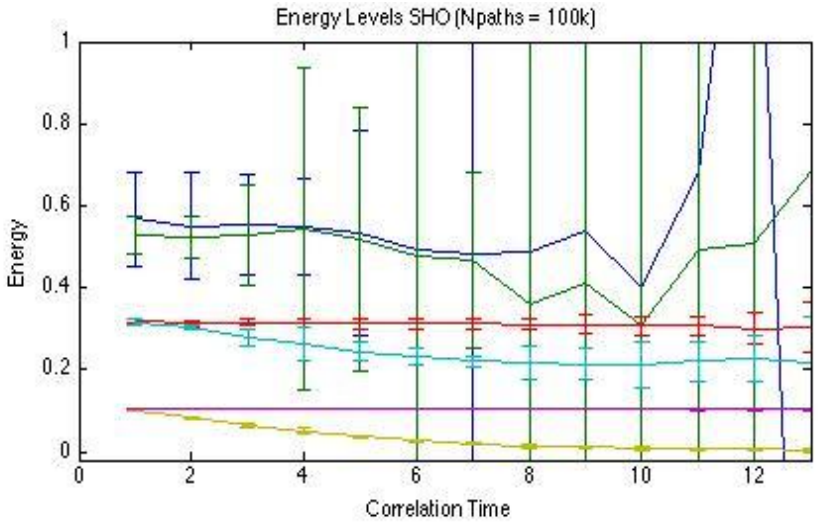
Correlation Calculation Benchmarks

- Single correlation (C_{11}) being generated for various values of tau max
- GPU is much slower for this calculation
- Moral: choose the right part of the algorithm to parallelize on the GPU

Max correlation time	CPU (seconds)	GPU (seconds)
128	4.033	8.053
256	4.718	12.825
512	6.004	22.042
1024	8.660	44.722

GPU Results


Energy Levels SHO (Npaths = 1mil)
Energy
Correlation Time
0
0.2
0.4
0.6
0.8
1
0
5
10
15
20


Energy Levels SHO (Npaths = 100k)
Energy
Correlation Time
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10
12

Conclusion

- Method works well for HO
- Errors grow significantly for the Double Well
  - adjacent energy levels are closer
- Path generation can be GPU accelerated
  - Correlation calculations too probably
- MCMC is not limited to the ground state

References

- The papers linked to from the course webpage for the final
- Good quick description of the jackknife procedure: http://www.physics.utah.edu/~detar/phycs6730/handouts/jackknife/jackknife/jackknife.html

Questions?