Institute of Physics, Belgrade
Scientific Computing Laboratory

Scientific Computing Laboratory

Path Integral MC @ SCL

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Who are we and what we do?

- Scientific Computing Laboratory of the Institute of Physics, Belgrade, http://scl.phy.bg.ac.yu/
- Numerical simulation of complex physical systems:
  - Path integrals in Quantum Field Theory and Condensed Matter
  - Granular Materials
  - planetary systems formation
  - Strongly correlated quantum systems
  - Dynamics of networks

Grid Infrastructure @ SCL

- Partners in EGEE-II and SEE-GRID
- EGEE and SEE-GRID LCG-2_7_0 Grid Site AEGIS01-PHY-SCL
- 100 CPUs on WNs – Xeons on 2.8 GHz with 1 GB of RAM
- Configured services: UI, CE, SE, MON, BDII, RB, PX
- VOMS for AEGIS VO (Academic and Educational Grid Initiative of Serbia)

AEGIS01-PHY-SCL

Path Integral Formalism

- General framework for all quantum theories introduced by Richard Feynman
- Specially suited for Monte Carlo
- Numerical calculation of path integrals is one of the most challenging problems (e.g. QCD simulations)
- All observables (expectation values) can be represented as some path integrals

Path Integrals at large

- They can be thought of as multiple integrals with infinitely many integrals, or as integrals over all possible trajectories/configurations
- Expectation values are calculated using weights of the type e^{-S}
- Numerically they are calculated as limits of different discretizations
- Typical convergence is slow - 1/N
- Important problem – speedup of the convergence by improving the action *S*

Ordinary Integrals (1)

- Definition

$$I[f] \equiv \int_0^T f(t)dt = \lim_{N\to\infty} I_N[f]$$

$$I_N[f] = \sum_{n=1}^N f(t_n)\epsilon_N$$

$$\epsilon_N = T/N \qquad t_n = n\epsilon_N$$

- Bad for brute force numerical calculations

$$I_N[f] = I[f] + O(1/N)$$

Ordinary Integrals (2)

- To analytically solve even the simplest integrals you needed to:
  - Find useful discretization
  - Do general N-fold sum
  - Do the continuum limit
- Euler's summation formula
  - Speeds up convergence to the continuum limit as fast as you want
  - Wasn't of much use numerically – no computers in the 18th century
  - Pointed to an underlying simplicity – precursor to integration theory
- Riemann's integration theory

Euler's formula (1)

- Discretization is not unique. Instead of $f(t)$ we construct an equivalent function $f^*(t;\epsilon_N)$:

$$f^*(t;\epsilon_N) \to f(t) \qquad \text{(in continuum limit)}$$

such that

$$I_N[f^*] = I[f] \qquad \text{(for all } N\text{)}$$

Euler's formula (2)

- Step 1: $f(t)=1$

$$I_N[1]=\sum_{n=1}^{N}\epsilon_N=T$$

thus f^*-f depends only on $\dot{f},\ddot{f},\ldots$

- Step 2: $f(t)=t$

$$I_N[t]=\sum_{n=1}^{N}t_n\epsilon_N=\frac{T^2}{2}+\frac{T^2}{2N}$$

$$I_N[t-\tfrac{\epsilon_N}{2}]=\frac{T^2}{2}$$

thus $f^*-f+\frac{\epsilon_N}{2}\dot{f}$ depends only on $\ddot{f},\ldots$

Euler's formula (3)

- Step 3: $f(t) = t^2$

$$I_N[t^2] = \sum_{n=1}^{N} t_n^2 \epsilon_N = \frac{T^3}{3} + \frac{T^3}{2N} + \frac{T^3}{6N^2}$$

$$I_N[t^2 - \epsilon_N t_n - \tfrac{2}{3}\epsilon_N^2] = \frac{T^3}{3}$$

thus $f^* = f - \frac{\epsilon_N}{2}\dot{f} - \frac{2\epsilon_N^2}{3}\ddot{f} + \ldots$

- etc.

Euler's formula (4)

- Therefore

$$\int_0^T f(t)dt = \sum_{n=1}^N f(t_n)\epsilon_N -$$

$$-\frac{\epsilon_N}{2}\sum_{n=1}^N \dot{f}(t_n)\epsilon_N - \frac{2\epsilon_N^2}{3}\sum_{n=1}^N \ddot{f}(t_n)\epsilon_N + \ldots$$

- We denote the first p terms of f^* by $f^{(p)}$. Then

$$I[f] = I_N[f^{(p)}] + O(1/N^p)$$

Path integrals (1)

- Amplitudes are the $N \to \infty$ limit of

$$A_N(a,b;T) = \left(\frac{1}{2\pi\epsilon_N}\right)^{\frac{N}{2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

- Action $\quad S = \int_0^T dt\, \left(\frac{1}{2}\,\dot{q}^2 + V(q)\right)$

- Naive discretized action

$$S_N = \sum_{n=0}^{N-1} \left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N V_n\right)$$

$$\delta_n = q_{n+1} - q_n \qquad V_n = V(\bar{q}_n) \qquad \bar{q}_n = \frac{1}{2}(q_{n+1} + q_n)$$

Path integrals (2)

- Goal: to construct equivalent discretized effective action

$$S_N^* = \sum_{n=o}^{N-1} \left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N W_n^* \right)$$

such that

$$A_N^*(a,b;T) = A(a,b;T)$$

- This is done up to p=10

P=3 example

- The level p=3 solution for S^* is

$$g_0 = V + \epsilon_N \frac{V''}{12} + \epsilon_N^2 \left[-\frac{V'^{\,2}}{24} + \frac{V^{(4)}}{240} \right]$$

$$g_1 = \frac{V''}{24} + \epsilon_N \frac{V^{(4)}}{480}$$

$$g_2 = \frac{V^{(4)}}{1920}$$

- Similarly for higher levels p. Note that the level p solution satisfies

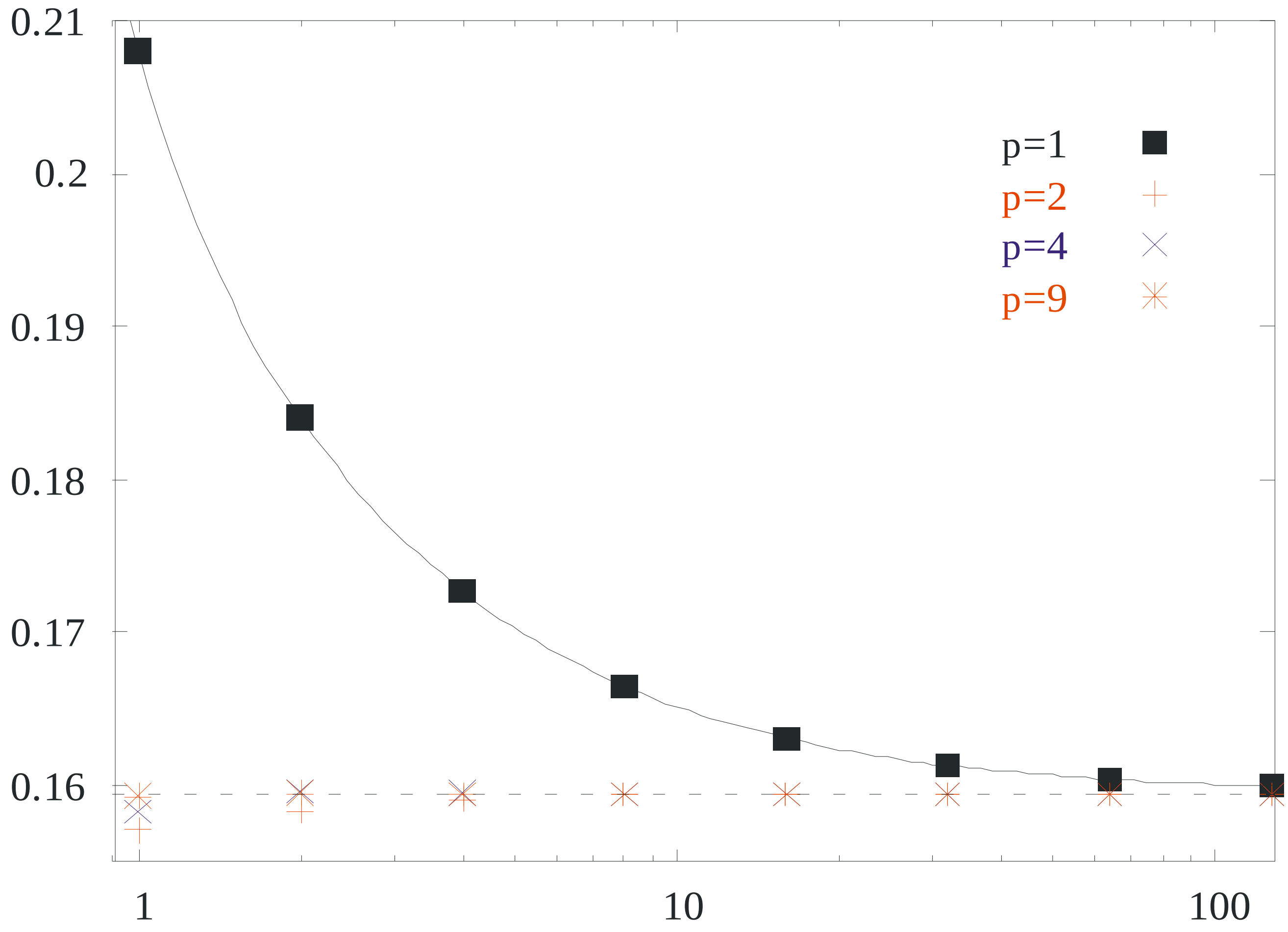
$$A(a,b;T) = A_N^{(p)}(a,b;T) + O(1/N^p)$$

  This is the Euler summation formula for path integrals.

MC code

- Serial and MPI code developed and tested
- Executed as an MPI application on MPI enabled sites supporting SEE-GRID and AEGIS VO
- Communication minimal – just at the beginning and at the end
- DAG job maybe the solution for porting on grids
- Code available on our web site

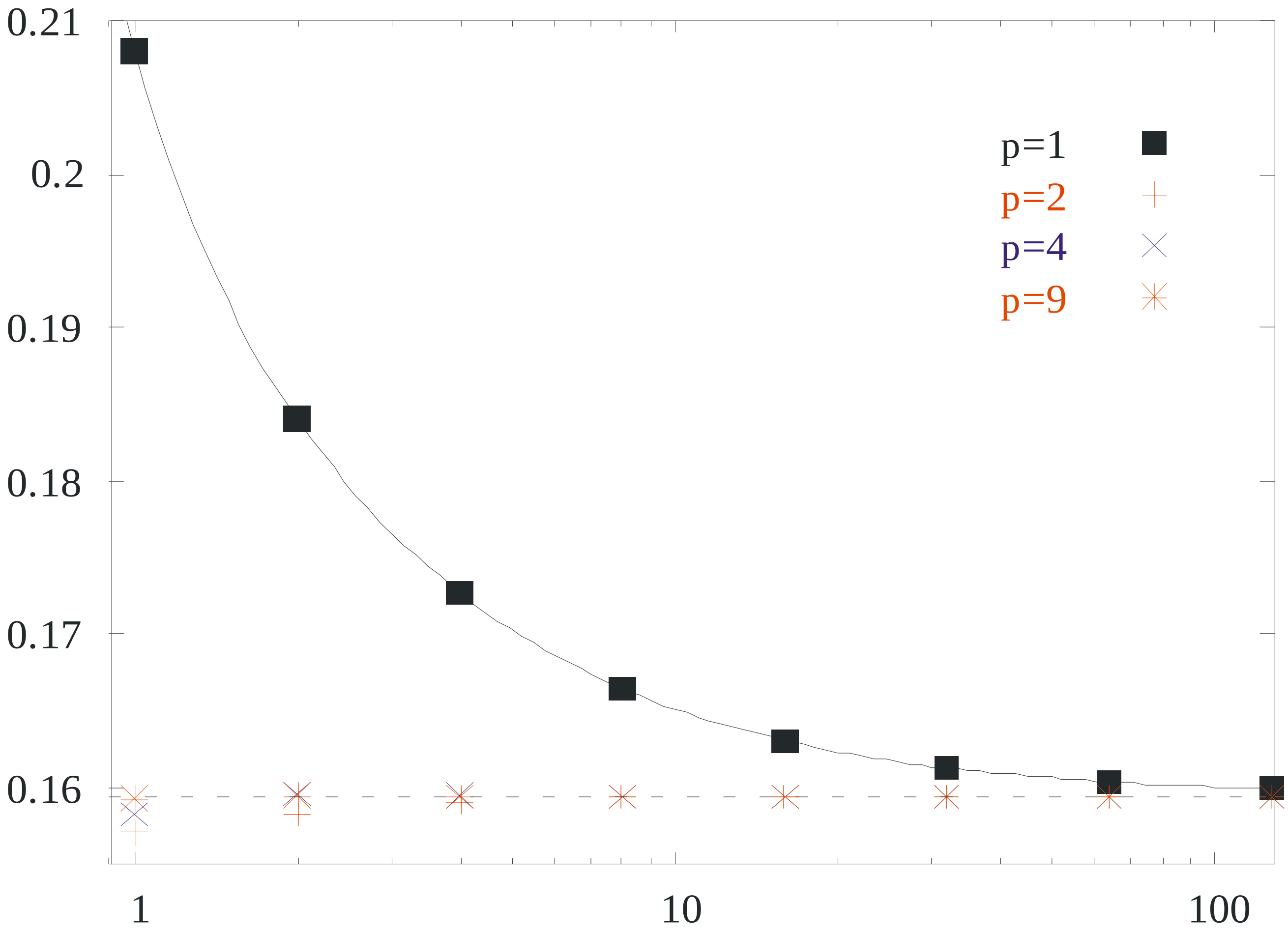
Numerical results (1)



Anharmonic oscillator with quartic coupling

$g = 1,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 10^7$

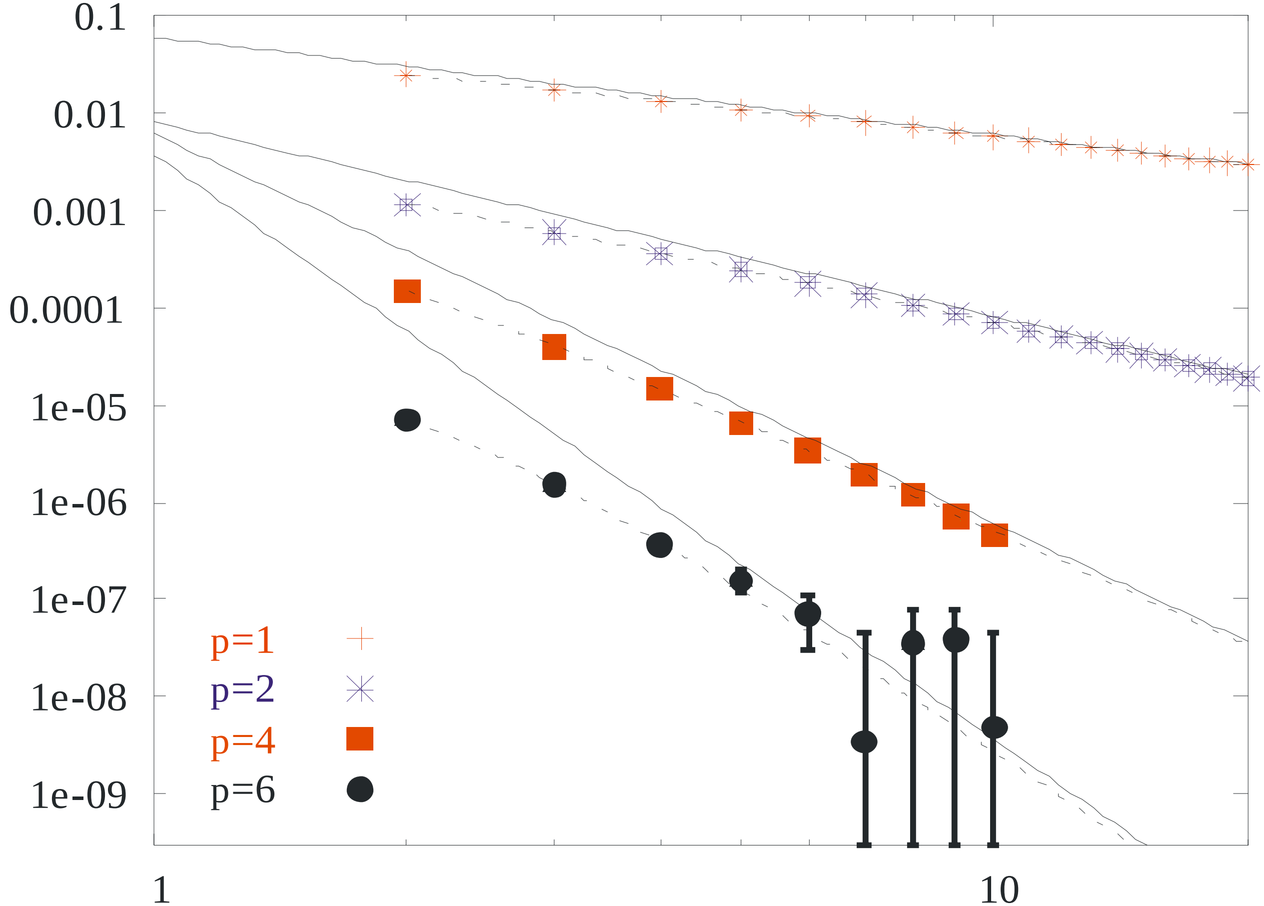
Numerical results (2)



Modified Poeschl-Teller potential

$$\alpha = 0.5,\ \beta = 1.5,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 9.2 \cdot 10^7$$

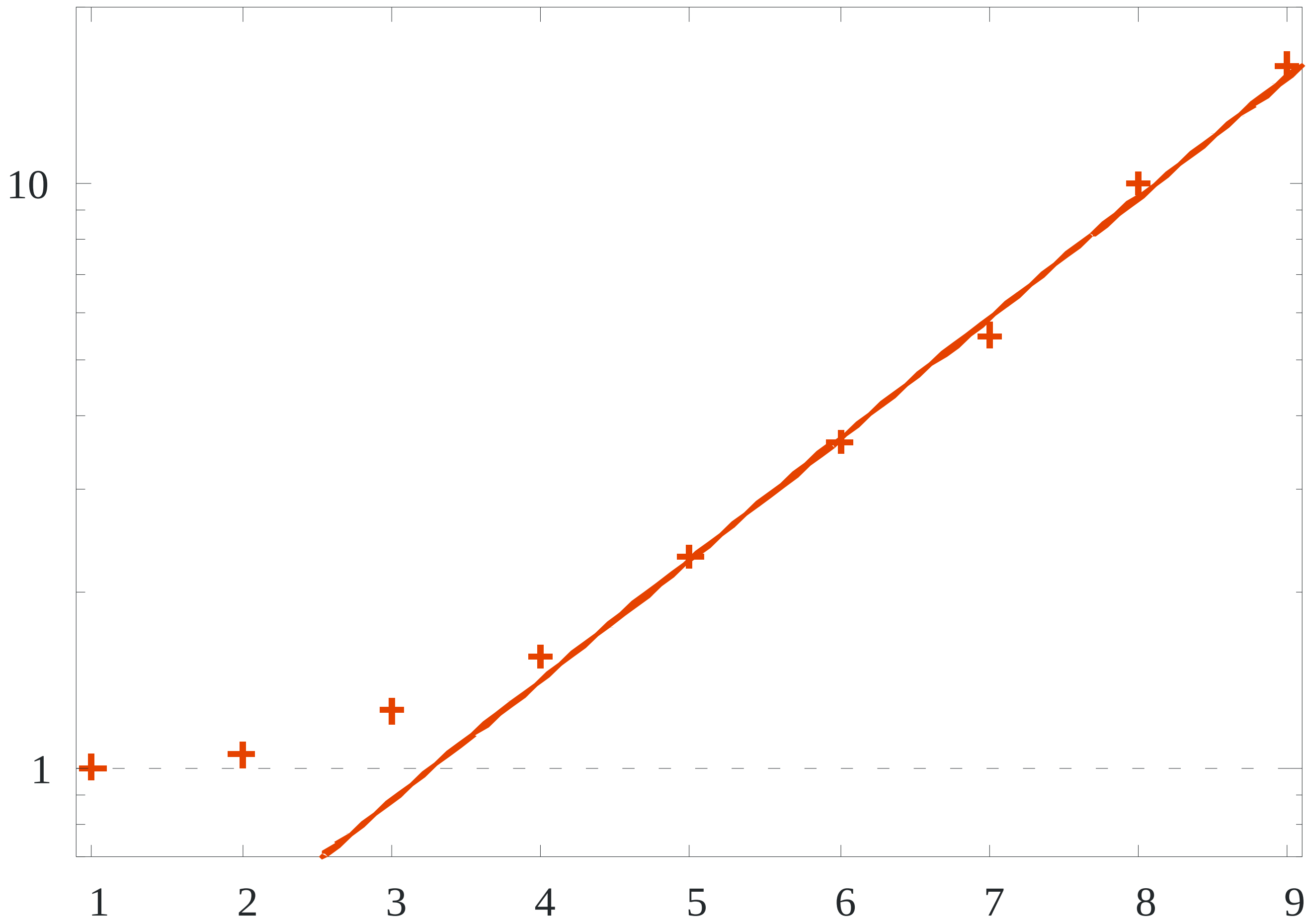
Numerical results (3)



Errors for anharmonic oscillator with quartic coupling

$$g = 1,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 9.2 \cdot 10^9\ (p = 1, 2),$$
$$N_{MC} = 9.2 \cdot 10^{10}\ (p = 4),\ N_{MC} = 3.68 \cdot 10^{11}\ (p = 6)$$

Numerical results (4)



Relative increase in computing time as a function of p

Discussion (1)

- The general path integral calculation is now speeded up by many orders of magnitude.
- However, it still takes a lot of CPU time to run real-life simulations
- This implies that porting of our MC code to the grid is necessary

Discussion (2)

- Extensions to many non-relativistic particles in d dimensions as well as to field theories in $d>1$ are in progress.
- Higher dimensional analogues of the integral equation are not a problem to derive. The algebraic recursive relations will be more complex and this could practically limit us to smaller values of p.

References (1)

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References (2)

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