Lanczos method in High-Performance Computing

Agenda

- Introduction, linear algebra recap.
- The Power method
- Krylov subspace
- Lanczos method

Introduction

High performance computing numerical analysis

States: Vectors in Hilbert space

Measurements: Linear Operators in the Hilbert Space

For example in Quantum Chromodynamics

$$S^{QCD} = \int d^4 x \bar{\psi}(x) D \psi(x) + \beta^{-1} \operatorname{tr} F(x) F(x)$$

Fermion states are represented by complex vectors

$$\Psi(x, y, z, t, a, \alpha)$$

a represents color, α spin

Observables are Correlation functions: Expectation values of operators

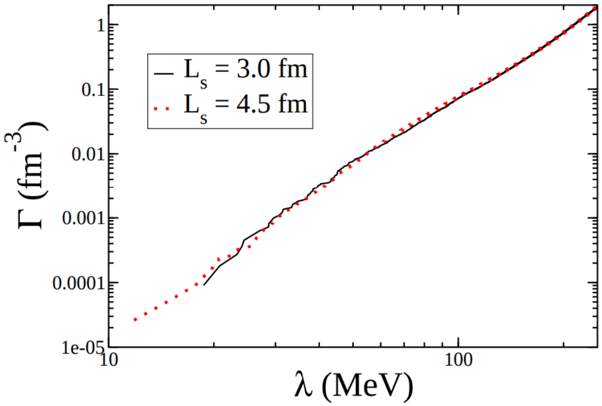
Spectrum of D

Eigenvectors

$$D\psi = \lambda\psi$$

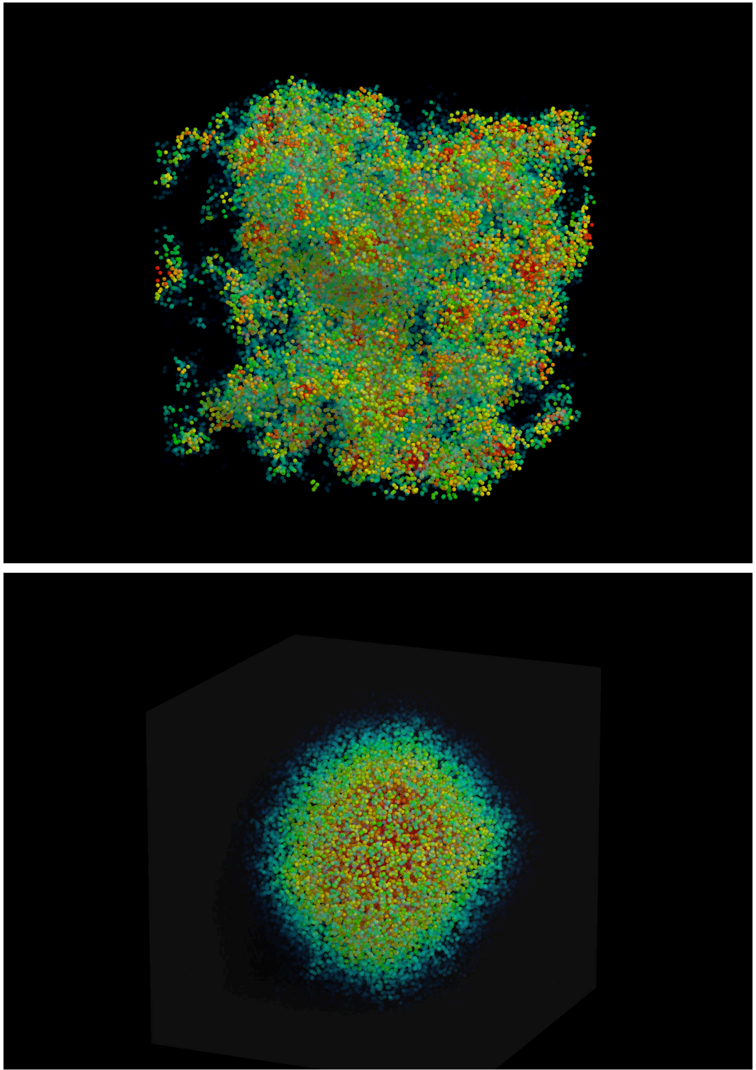
λ is a number

Spectral density



Low eigenvalues are important

Low eigenmodes of D



How to differentiate localized-delocalized eigenvectors ?

- Eigenvectors are normalized

$$\sum_x |\psi(x)|^2 = 1$$

- What happens when we sum the moments of the wave-functions?

$$\sum_x |\psi(x)|^4 = ?$$

- In the delocalized case $\psi(x)$ does not depend on x.

$$\sum_x |\psi_0|^2 = V\psi_0^2 = 1$$

- Thus for the second moment we get

$$\sum_x |\psi_0^4|^2 = V\psi_0^4 = 1/V$$

The Power method

- Given x_0, A
- Compute x_1=Ax_0
- x_2=Ax_1
- x_3=Ax_2
- x_4=Ax_3
- Till
- x_k=Ax_k-1 approaches the dominant eigenvector

Lanczos method

Eigenvalues of the Krylov subspace

$$\square(A, v_0) = \{v_0, Av_0, A^2v_0, A^3v_0, \cdots, A^nv_0\}$$

Approximate the eigenmodes of A using the Krylov subspace

D is sparse

n is typically small

Storing the subspace is expensive

Lanczos method

- vector `v_1` be an eigenvector with `| v_1 |- = 1`
- beta0 :=0 v0:=0
- for k=1,2,3,… do
- w:= A*v_k
- alpha_k := (v_k*w)
- T_k,k := alpha_k
- Diagonalize T^(k) and stop if e_n converges
- w := w - beta*(k-1)v*(k-1)-alpha_kv_k
- for l=1,2,…,k-2; do
- w:=w-v_l(v_l*w)
- end for
- beta_k=sqrt(w*w)
- v_(k+1)=w/beta_k
- T_{k,k+1}:=beta_k
- T_{k+1,k}:=beta_k
- end for

Thick Restarted Lanczos

- 1: vector v1 be an arbitrary vector with ||v1|| = 1
- 2: kx := 1
- 3: for l = 1, 2, 3, … do
- 4: for k = kx, kx + 1, kx + 2, …, lm – 1 do
- 5: w := Hvk
- 6: αk := (vk · w)
- 7: Tkk := αk
- 8: Diagonalize T(k) and stop if e_n converges
- 9: for l = k, k – 1, · · · , 2, 1 do
- 10: w := w – vl(vl · w)
- 11: end for
- 12: βk := |w|
- 13: vk+1 := w/βk
- 14: Tk,k+1 := βk, Tk+1,k := βk
- 15: end for
- 16: Construct a new T1(ls+1) matrix and v1, · · · , vls+1 for restart
- 17: kx := ls + 1
- 18: end for

Implementation details

- Question CPU or GPU, which parts are most computationally expensive
- Application of the operator
- Linear algebra
- The following kernels have to be implemented
- paxyb : y:=ax+b
- scalar product of two vectors
- updating the lanczos basis