Andromeda : a few-body plane-wave calculator

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High dimensional Search with Low dimensional output

Digital Quantum Electrons

- No Artificial Intelligence!
- No Machine Learning!
- No Quantum Computing!
- Just classical computing!!?!

Component separation

Reduction to one spacial dimension

Component separation

Sums Of Products = Sum of many — F(x) G(y) H(z)

Given a function

Analytically Formulate exact digital Matrix

$$x^2 + y^2 + z^2 = r^2$$

Pythagorean Theorem

Vector magnitude is separable

$$e^{-x^2} \times e^{-y^2} \times e^{-z^2} = e^{-r^2}$$

Gaussian is also separable

$$f(s) = \int_0^\infty \frac{g(t)}{2\sqrt{t}} e^{-st} \mathrm{d}t = \int_0^\infty g(\beta^2) e^{-s\beta^2} \mathrm{d}\beta,$$

Laplace Transform of your favorite interaction

Expressed as a sum of Gaussians

$$\int_{-1}^{1} f(x)\, dx \approx \sum_{i=1}^{n} w_i\, f(x_i),$$

Lagendre Quadrature the integral

Lazy like, express as G with integral index

$$\mathcal{D}(G)_{nm} = \int_{-\infty}^{\infty} \mathrm{d}x \{ \int_{-\pi}^{\pi} \mathrm{d}p e^{\imath p(x-n)} \int_{-\pi}^{\pi} \mathrm{d}k e^{\imath k(x-m)} \} \mathcal{F}(G)(q) e^{\imath q x}$$

Digitize Gaussian

Any basis is possible but we chose the Sinc as the most local version of plane-waves

Exchange is expressible as SOPs,
the few-body computations require this type of term

Average error of a few nanoHartree for
2-body Coulombic interactions

Core Matrix Vector Multiply

$$M_{n_1 n_2 n_3 m_1 m_2 m_3} = \sum_{\lambda} X^{\lambda}_{n_1 m_1} Y^{\lambda}_{n_2 m_2} Z^{\lambda}_{n_3 m_3}$$

$$v_{n_1 n_2 n_3} = \sum_{\mu} x^{\mu}_{n_1} Y^{\mu}_{n_2} Z^{\mu}_{n_3}$$

GEOMETRIC GROWTH

$$Mv = \sum_{\lambda\mu} (X^{\lambda} x^{\mu})(Y^{\lambda} y^{\mu})(Z^{\lambda} z^{\mu})$$

Essential Problem

- Component separated terms geometrically increase in number under matrix-vector multiplication

Solution

ALTERNATING LEAST SQUARES

Algorithms for Numerical Analysis in High Dimensions

Gregory Beylkin, Martin Mohlenkamp

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Lifting the curse of dimensionality

"The N^3 problem has become a 3N problem."

- –Anders Niklasson @ Los Alamos National Laboratory

Elementary…

- IBM Qbox can compute upwards of 200 Teraflops on 65K cores
- 3 Gigaflop per core

- Basecamp of 40 Petabyes,
- 34,009 s per iteration on 36 cores
- That’s 32 Gigaflop per core
  - 10x algorithmic speedup
- @ 0.1 % holistic error

Timings to run a quantum 3-body matrix-vector multiply

An exa-sample with L = 100

SOP Hamiltonian Lithium	SOP wave function Vector state	Matrix-vector multiply on 100 cores
few seconds	Loads in few seconds	few hours
few Gb	few Gb	hundred Gb

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