Update 25.02.2022

QUBO processing improvements and preparation for the DPG

Spataro David
Hamburg, 25.2.2022

QUBO main parameters

Parameters set via loading yaml file

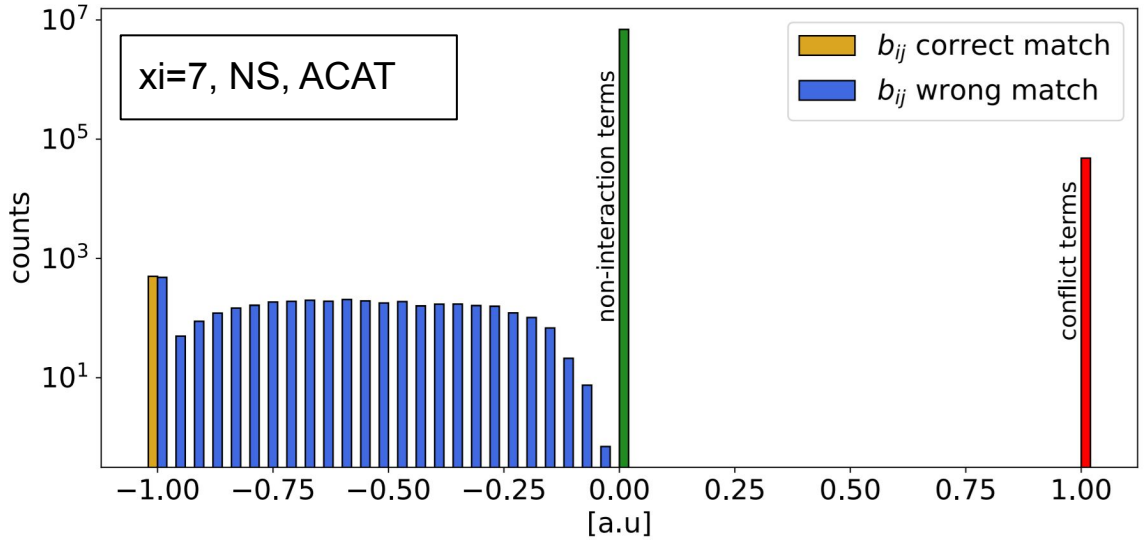
```yaml
---
ansatz parameters:
  name: "TwoLocal"
  circuit depth: 2
  num qubits: 7
  rotation blocks: "ry"
  entanglement blocks: "cx"
  entanglement: "circular"


solver parameters:
  mode: "VQE ideal qasm sim"
  optimizer: "NFT"
  maxiter: 5000
  seed: 42
  shots: 10
  optimization level: 2

QUBO solving:
  search depth: 1
  num qubits: 7
  compare to eigensolver: True
  vqe: True

tabu usage:
  function:  "simple tabu"
  initial: True
  loopwise: True
  final: True
```

- Ansatz:
  - name implies on how the program will handle it
  - “Adaptive Locally Connected” will trigger a dynamic ansatz approach, which takes into account the connection between triplets/qubits, only “strong connection” at the moment, later a “weak connection” will be implemented too
- Solver:
  - different modes, Numpy Eigensolver, VQE with/out noise, IBM…
  - more parameters can be added, but that’s for fine-tuning things
- QUBO solving:
  - solving mode, tabu usage, search depth
- tabu usage
  - function (adding new function objects)
  - specify when tabu search should be used

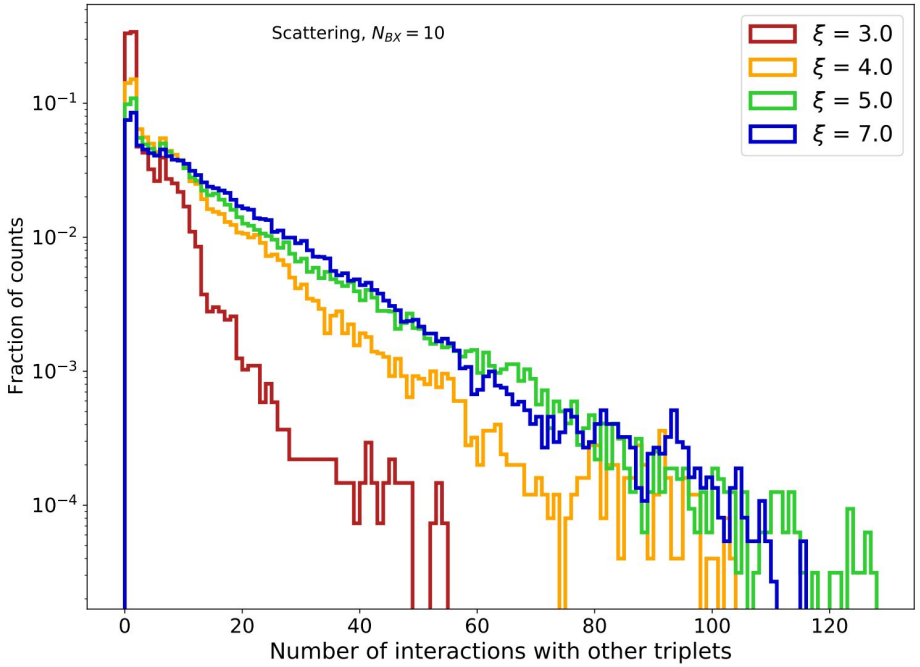
Hamiltonian Energy Calculation I

From Matrix operations to summation

- Before: Energy calculation via matrix, size of matrix is #triplets x #triplets → 250MB for 1800 triplets originating from ~800 tracks on a low hit density sample (xi = 3) ~99% of matrix has a zero as entry



- Number of interactions seem to “saturate” at some point, so we still expect a nearly empty matrix for high xi values



Hamiltonian Energy Calculation II

From Matrix operations to summation

- Now: Store information about interaction inside the triplet object, e.g:
  - triplet.interactions = {1: -0.67231, 345: 1, 285: -0.93425} → no zeros appear, huge decrease in data size
  - disk space needed decreased from 250MB to < 1MB and not increasing quadratically anymore!
- energy is calculated by going through the triplets and directly calculating each energy term, very fast, less than half a second per 1800 triplets
- tabu search speed is also increased by that
- possible for ~65k particles just the way it is
  - 18M Doublets, 3h 45 min , 2GB → better split into overlapping areas and solve them

Next tasks

Making “experiments”

- Framework now reworked → making a roadmap, including
  - different settings of qubo coefficients
  - xi =3, 4, 5, 6
  - number of qubits = 2, 3, 5, 7, 10, 16
  - Numpy Eigensolver
  - Two Local (different circuit depths)
  - “Adaptive Locally Connected“ → for DPG
    - two different types