ANOTHER SOLUTION FOR AMBER QM/MM MD SIMULATION: SEAMLESS INTEGRATION WITH SANDER & QUICK

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OUTLINE

- AMBER QM/MM calculation
- QUICK & AMBER integration
  - None Periodic Boundary
  - PBC - Ewald and PME

CURRENT AMBER QM/MM MD

- Semi-empirical: implemented by SQM, support AM1, PM3, DFTB...
- NOT fully parallel implementation
- Ewald summation and PME is available
  - *Kwangho Nam, Jiali Gao, and Darrin M. York, J. Chem. Theory. Comput., 1, 2-13, (2005).

CURRENT OF AB INITIO AND DFT QM/MM WITH AMBER

- Pupil
  - Pros: powerful, a universal interface for multiple QM and MM software
  - Cons: requires configuration. Based on file exchange.
- Terachem
  - Pros: Powerful, support GPU. Sander centered.
  - Cons:Based on file exchange. Not sander based

WHAT ABOUT QUICK & AMBER INTEGRATION?

- **Pros:**
  - **inherently sander based, not based on file exchange**
  - **easy to use. similarly configuration to original Semi-empirical method**
- **Cons:**
  - **not powerful enough.**

HOW TO USE AMBER-QUICK INTERFACE?

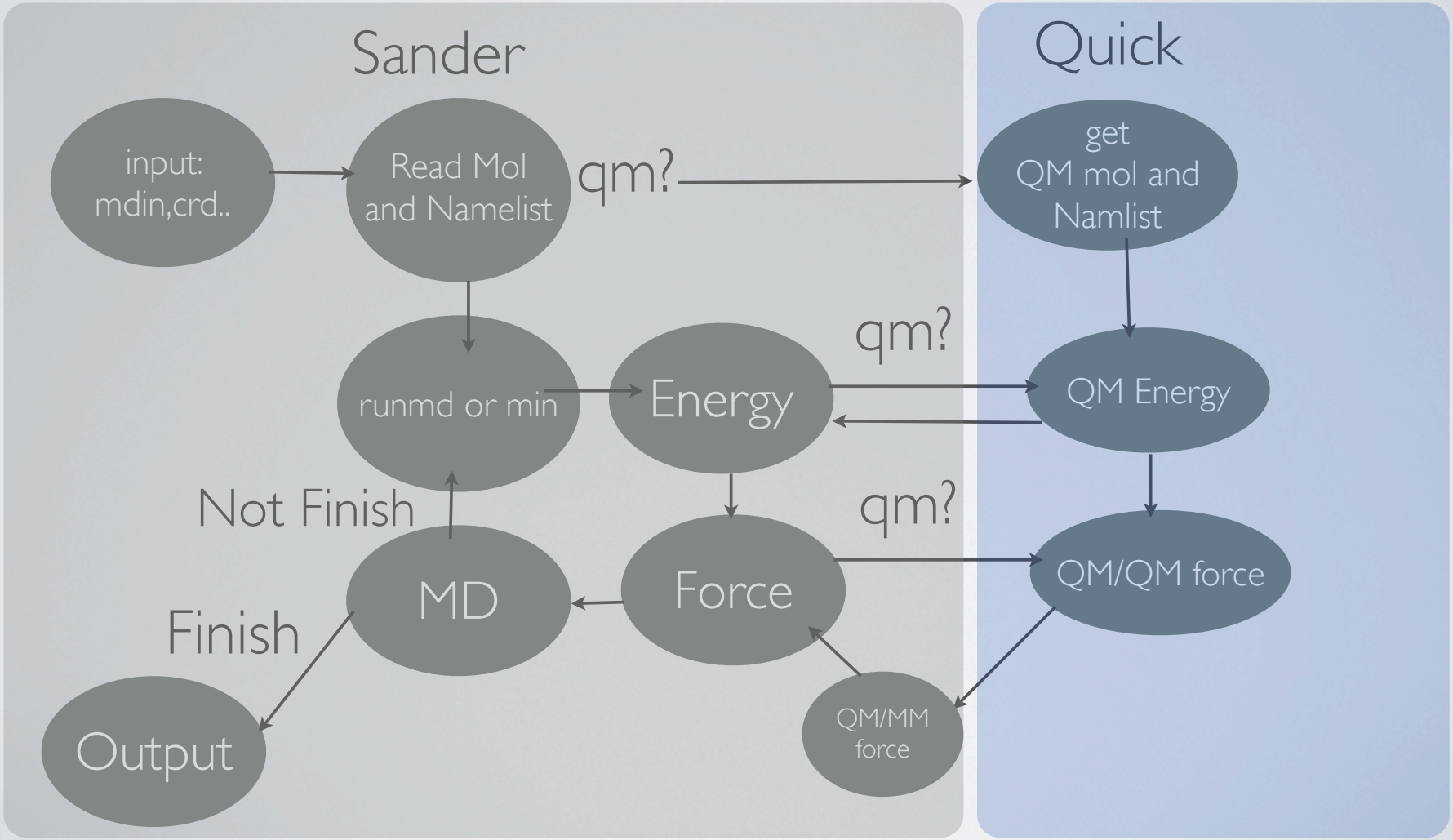
AM1:

```
 &qmmm
  qmmask=':1-2',
  qmcharge=0,
  qm_theory="AM1"
  ...
```

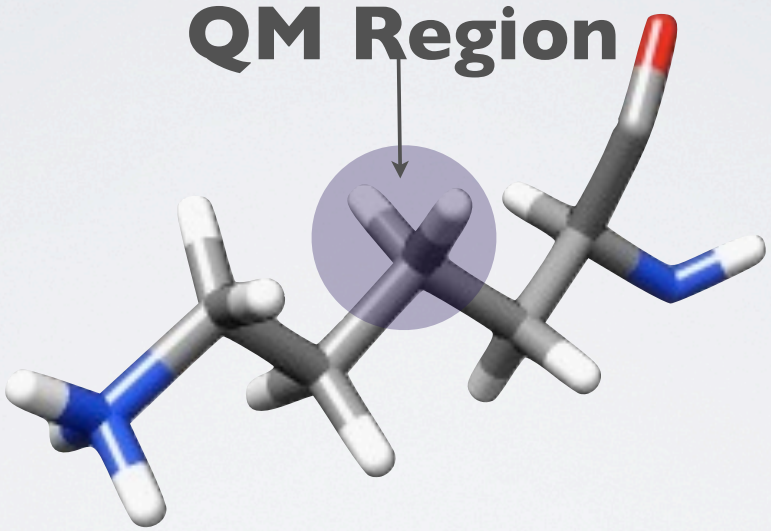
HF:

```
&qmmm
  qmmask=':1-2',   -> define QM region
  qmcharge=0,      ->QM charge
qm_theory="HF"->Theory:HF,MP2,DFT
  basis="6-31g"     ->[new namelist]
  ...                    default: sto-3g
```

IMPLEMENTATION



TEST CASE (NONE PERIODIC BOUNDARY CONDITION)



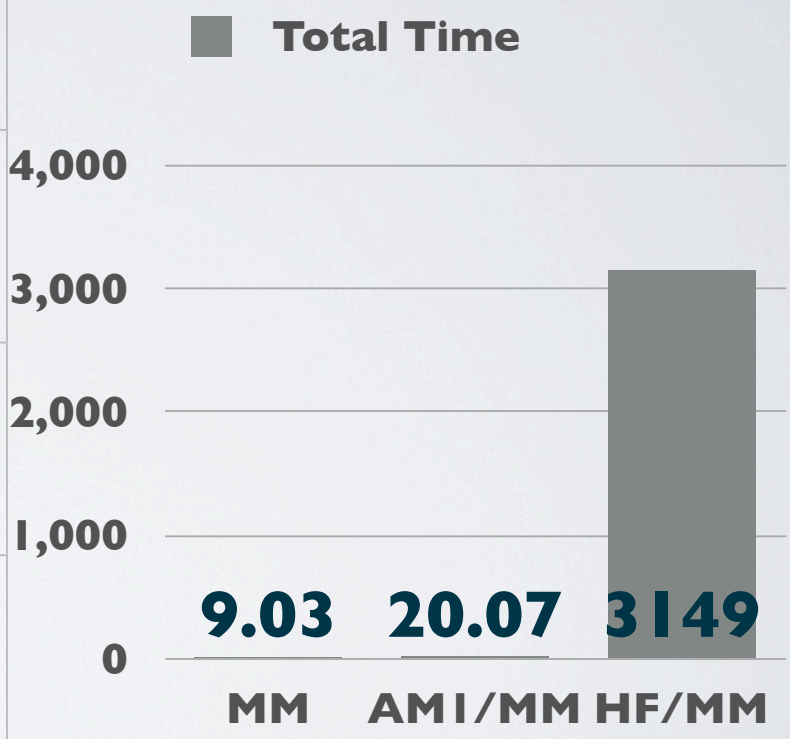
lysine, nstlim=20000, 2ps, 22 Total atoms, 5 QM atoms, STO-3g

RMS: HF VS AM1


"lysine_md.rms.save.AM1"
"lysine_md.rms.save.HF"
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
500
1000
1500
2000
2500
3000
3500
4000

TIME COMPARISON

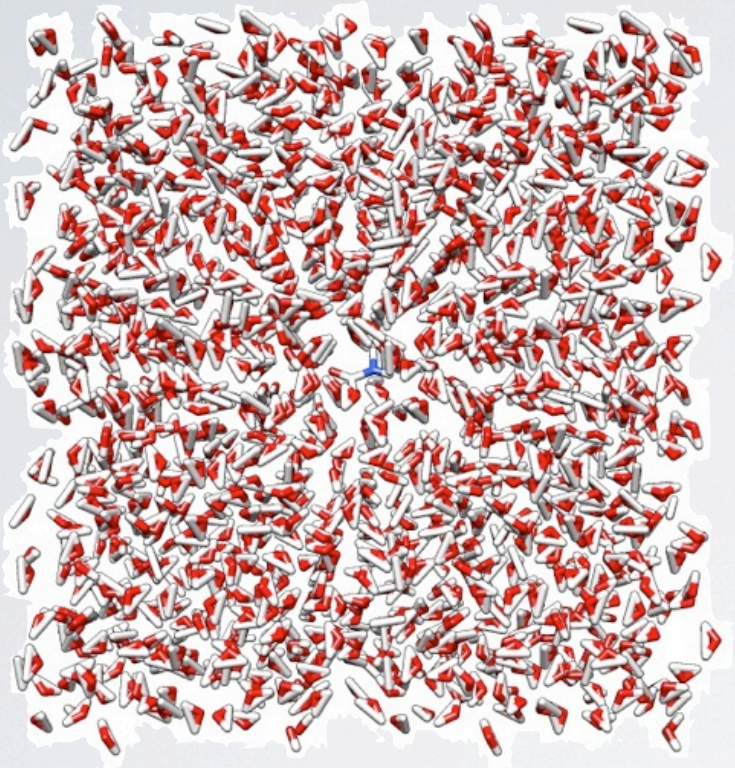
	MM	AM1/MM	STO-3g-HF/MM
Total Time/s	9.03	20.07	3149
Per Step/ ms	0.45	1.00	157.45
ns/day	191.35	86.09	0.55



nstlim=20000, 2ps, 22 Total atoms, 5 QM atoms

TEST CASE (PBC)

- **Ewald Summation and PME**
- **QM/MM Ewald Summation and PME**

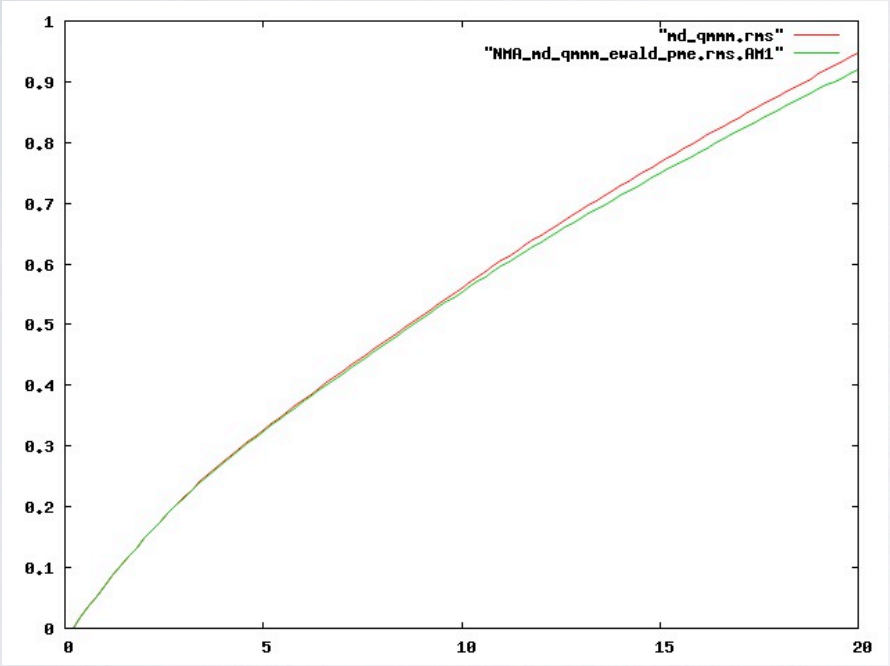


N-methylacetamide(NMA)
QM region: NMA, 12 atoms
MM region: water, 4578 atom

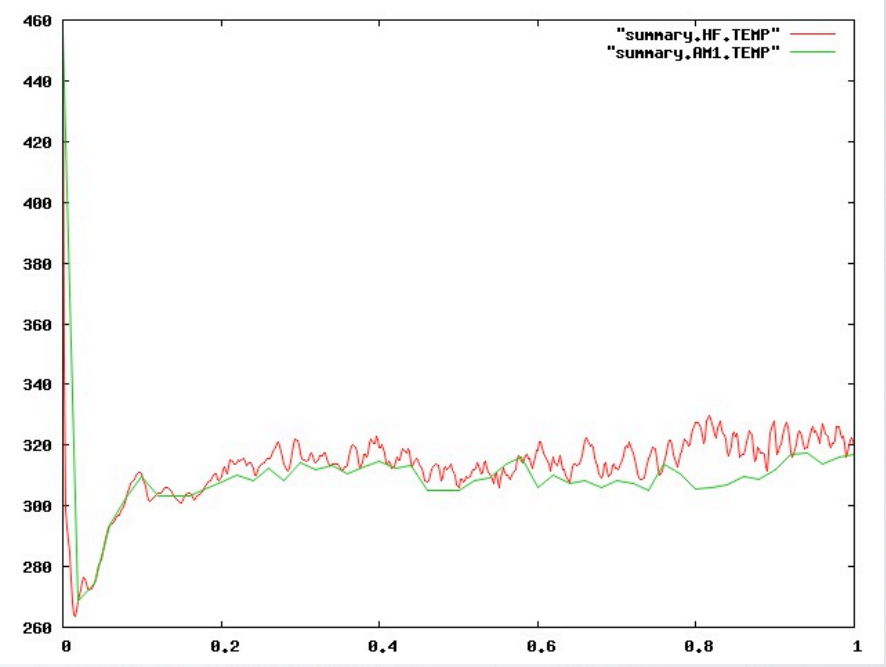
400 steps, 0.8ps

HF/sto-3g time:
10447 ms/step
AM1 time:103 ms/step

RMS


"md_qmmm.rms"
"NMA_md_qmmm_ewald_pme.rms.AM1"
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20

TEMP


"summary.HF.TEMP"
"summary.AM1.TEMP"
460
440
420
400
380
360
340
320
300
280
260
0
0.2
0.4
0.6
0.8
1

PARALLEL

- **QUICK and AMBER inherently support MPI**
- **Users can select sander+quick.MPI and sander.MPI+quick.MPI**
- **test case is under test.**

8000 steps	1	2	4	8
second/ step	4.008	2.739 (68%)	1.859 (47%)	1.565 (39%)

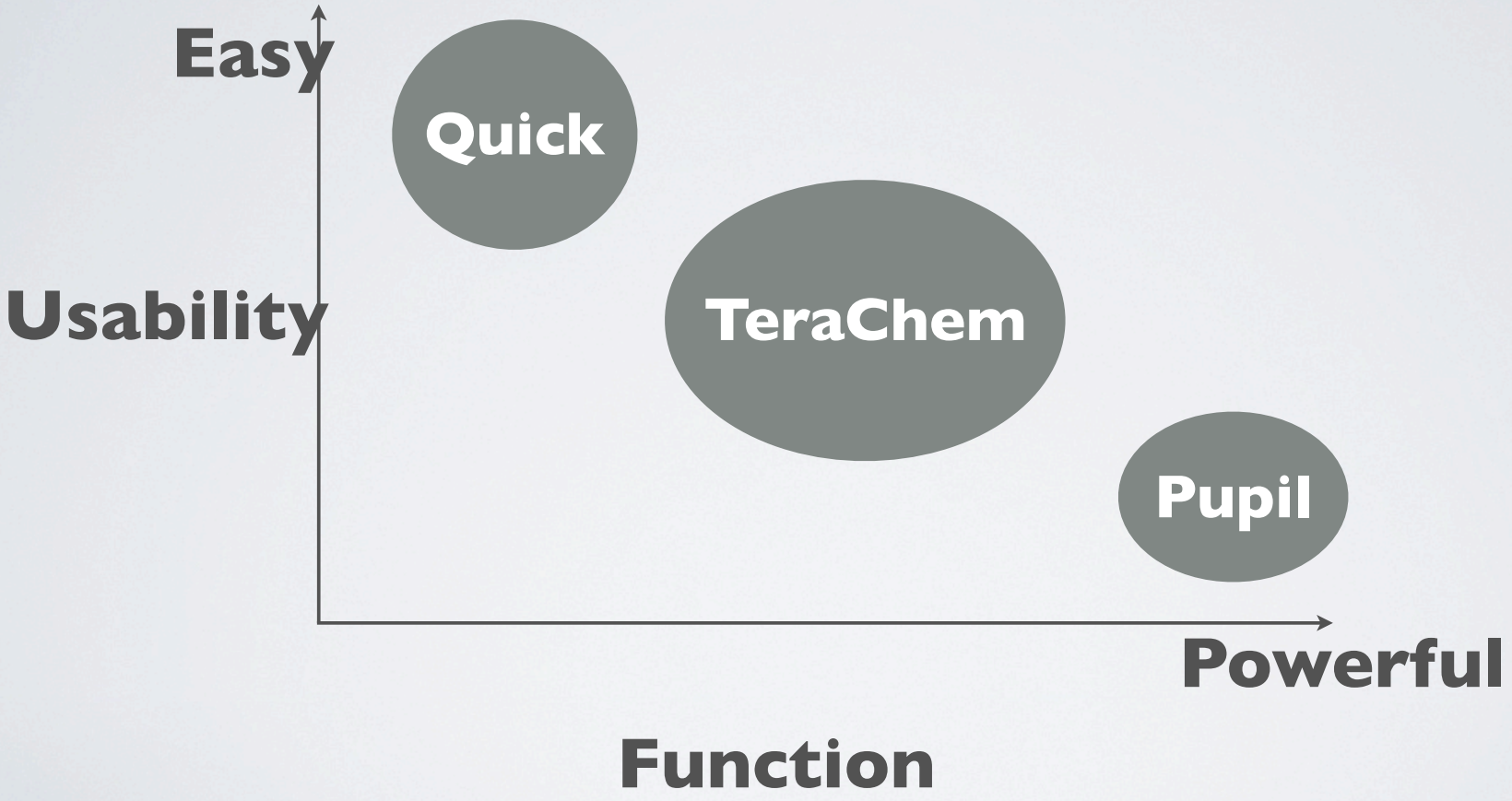
LIMITATION

- **Limited QM theory is supported: HF and DFT (limited functional)**
- **No GB**
- **SHAKE fails for unknown reason**

IN PROGRESS

- More QM thoery (MP2, DFT, ab initio Div & Con...)
- GB
- GPU

A VISIBLE LOOK: COMPARISON



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- Merz Group

THANK YOU!