Tinker Software Workshop 2018

The University of Texas at Austin, June 2-4, 2017

All meetings are in BME 3.204

(BME Building on Google map: https://goo.gl/maps/DgoBYwGehqA2)

● June 2nd, Saturday, (9:00-11:45 am & 13:30-16:30 pm)

1) Code Bases & Programming Models (Ponder)

(Approximately 10 minute presentation per topic, plus discussion)

Topics: Current status of various code bases and what have been changed since the last meeting

a) Tinker: Ponder
b) Tinker-HP: Piquemal
c) Tinker-OpenMM: Ren
d) OpenMM: Eastman
e) Amber & PMEMD: Case
f) CHARMM: Brooks
g) FFX: Schnieders
h) Q-Chem/EFP: Head-Gordon
i) MolSSI Intro and Database project: Jessica Nash

2) Algorithms & Methodology (Schnieders)

Topics: Very brief description of the method, applications, and current & future implementations

a) Polarization
iELSCF: Head-Gordon
OPT: Simmonett
TCG and beyond: Aviat
DC-JI/DIIS: Greg Beran or D. Nocito
Simplification of “d” and “p”: Simmonett

b) MD
Constant pH: Schnieders

Integrators: Lagardere
Integrators: Tuckerman
Best practice in implementing/choosing thermo & barostat

c) Sampling

Sampling OSRW: Wei Yang
Parallel-in-Time: Maday
Accelerated MD: Eastman
Steered MD: Piquemal

d) Models

Implicit solvent MIB-PB: Guowei Wei
ddCOSMO: Stamm
GK: Schnieders

QM/MM: Cisneros
QM/MM: Yihan Shan
QM/MM: Daniele Loco (AMOEBA embedding and QM/MD)
Filippo Lipparini (Gaussian interface)
PME for dispersion: Andy Simmonett

Metal ions/Sammer Varma

Automated Parameterization: Chris Ho
POLTYPE: Brandon Walker, torsion/implicit solvent
Coarse-grained RNA model: Sara Cheng

e) New Force Fields

Open Force Field: Michael Schauperl
SIBFA: Piquemal/Gresh
GEM: Cisneros
MPID: Brooks
AMOEBA2: Rackers/Ponder
AMOEBA+: water model Chengwen/Ren

3) Development over the next year (Part A)

a) Hardware (Piquemal)

CPU Vectorization: AVX512 speedups (Jolly)
CPUs/hybrid
GPUs: NVIDIA *vs*. AMD, CUDA *vs*. OpenCL vs OpenACC
Volta/Tensor core

~~IBM OpenPOWER~~ Something else? Swope/Rice

Programming Models: MPI 3.x, OpenMP 4.x
Hybrid CPU / GPU Code Multi-Platform Support

b) Software (Ponder)
Tinker (C++ vs. Fortran)
Tinker-HP
Tinker-OpenMM
Amber
Charmm
QM/MM (Gaussian, Q-chem)

Priorities for next year:
Support for Current Versions in Tinker of Existing Models/Force Fields (Amber, CHARMM, OPLS, *etc*.)
Support for New and Emerging Force Fields, esp. Polarizable Methods Algorithmics & new Mathematics / Physics
Support for free energy methods

● June 2nd, Saturday Dinner
(6:30 – 8:30 pm; dinner at the AT&T center in room PDR 1&2.)

4) Discussion & Social Hour(s)

Taco Bar 16
Smoked Brisket, Pork Carnitas, Tinga Chicken, Portobello Mushroom, Flour Tortillas, Lettuce, Tomato, Jalapeño, Cheddar, Sour Cream, Guacamole, Fire Roasted Salsa

● Sunday, June 3rd
(9-11:45 am; 1:30-4:30 pm)

5) Development over next year (Part B) (Ponder/Ren/Piquemal)
a) TINKER as the reference code; put new methods / code there first, and then move to TINKER-HP, OpenMM, etc.

b) Integration of the three Tinker code bases (merge at "TINKER 9" ?) Multiple versions of polarizable electrostatics, or a single version – ?? Not happening
c) Tinker 8, Tinker-HP, QI; Speed Comparisons Refactoring to enable MPI
d) PCG and TCG *vs*. DIIS on GPUs
e) Updated OSRW Versions; Lambda Derivatives, *d*U/*d*lambda; Soft-Core vdw & Electrostatics
f) QI implementation of multipoles
g) Refactoring to enable Domain Decomposition Tests of importance of dispersion PME (?)
h) Stay in sync with "Canonical" OpenMM Tinker-OpenMM branch with periodic merges
i) Develop new GPU code (CPU/GPU hybrid, AMD, Intel Phi) Free Energy Methods and Sampling
j) Free Energy Calculations; dual topology. Alchemical Perturbation (extensions of existing code) Thermodynamic Integration / Metadynamics
k) Double Precision (CPUs) *vs*. Mixed / Single Precision (GPUs) Does it matter? for which Problems?
l) QM/MM (Gaussian, LIChem, CHARMM, Q-Chem, others)
m) Trajectory Storage, Transport and Archiving; Binary file format(s) Compatibility with ptraj / Amber

6) Applications & Tutorials (Nerenberg/Schnieders)

a) UI/FFX (Schneiders/Ponder)
b) Classroom & Laboratory Exercises Wiki and /or User Forum for Questions
c) System set ups
d) Free Energy Simulations
FEP, BAR, MBAR, ΔH / ΔS QM / MM
e) pKa Calculations
f) Protein & Nucleic Acid
g) Small Molecule Crystal Simulations
h) Heavy Metal Ions

● **June 3rd, Sunday Dinner**
(Downtown Austin; 18:00-21:00 pm)

Parkside http://parkside-austin.com/
Roaring Fork http://roaringfork.com/

● **June 4th, Monday (BME 3.204, 9:00-11:30 am)**

7) GitHub / WebSites & License Issues

TinkerTools.org Site
Documentation, Regression Testing Tutorials

GitHub Site for each Tinker Code

Github usage/best practice: Josh/Andy

Version N-1 will be Publically Available
Public GitHubs will allow Free Download (including Companies). Private GitHubs with access for Developers
Free license/open source for academic and non commercial
Commercial license between Washington Univ., Univ. Texas-Austin and Sorbonne

8) Organization of Software Development

Software Developers
Core Developers Ponder / Ren / Piquemal, and parts of our groups Developers
Head-Gordon, Brooks, Cisneros, Schnieders, Yang, their groups, and other from this meeting
Contributors People from Outside this Meeting

Who is Going to Do What?

Development Targets Release Dates / Plans Publications and Reference

Tinker papers:

Tinker 8 publication by tinker/tinker-HP key developers
Tinker 9 publication, including all developers?

Participants:

Greg Beran	University of California, Riverside
Bernie Brooks	National Institutes of Health, NHLBI
Dave Case	Rutgers University
Sara Cheng	University of Texas, Austin
Andres Cisneros	University of North Texas
Tom Darden	OpenEye Scientific Software
Akshaya Das	University of California, Berkeley
Omar Demerdash	Oak Ridge National Laboratory
Peter Eastman	Stanford University
Nohad Gresh	Sorbonne Universite
Matthew Harger	University of Texas, Austin
Teresa Head-Gordon	University of California, Berkeley
Chris Ho	Drug Design Methodologies
Luc-Henri Jolly	Sorbonne Universite
Preston Keller	Kingdom Capital
Louis Lagardere	Sorbonne Universite
Filippo Lipparini	University of Pisa
Jacob Litman	University of Iowa
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