Tinker Software Developer Workshop

Washington University in St. Louis, 16-18 March 2017

● *Thursday, March 16th*

(Danforth University Center, Room 476, 8:30-11:30 & 13:00-16:00)

(1) Code Bases & Programming Models

(A) What Is (or Should be) Supported Now?

TINKER Codes	Tinker, Tinker-HP, Tinker-OpenMM
Support AMOEBA	FFX, PME-MD, CHARMM, OpenMM
Possibilities	NAMD, GROMACS, Amber GPU
Software Models	MPI, OpenMP, CUDA, OpenCL

(B) Code Base Presentations

(Approximately 10 minute presentation per topic, plus discussion)

Topics: What is Currently Implemented and Planned for the Coming Period?
Future Interaction with Tinker Community

Tinker	Ponder
Tinker-HP	Piquemal
Tinker-OpenMM	Ren
OpenMM	Eastman
CHARMM	Brooks
Amber & PMEMD	Case
FFX	Schnieders
Q-Chem/EFP	Head-Gordon

(2) Algorithms & Methodology

(Approximately 10 minute presentation per topic, plus discussion)

Topics: *Very* Brief Description of the Method, What is Currently Implemented and in which Codes, Current and Future Applications

Polarization: iELSCF	Head-Gordon
Polarization: OPT	Simmonett

Polarization: TCG	Aviat
Polarization: DC-JI	Ponder (Beran's new method)
Charge Penetration	Rackers
Charge Transfer	Ren; Head-Gordon
Polarization Models	TBD
Exchange-Dispersion	Rackers
PME for Dispersion	Pickard
Force Fields: GEM	Cisneros
Force Fields: SIBFA	Gresh
Integrators: SIN(R)	Tuckerman; Wang
Domain Decomposition	Pickard; Lagardere
Fast Multipole Method	Piquemal
OSRW	Yang
Symmetry / Crystals	Schnieders
Accelerated MD	Eastman
Thermostats / Barostats	Ponder
Generalized Kirkwood	Schnieders
ddCOSMO	Stamm
MIB-PB	G. Wei
Constant pH	Schnieders
Normal Modes / Analyt Hessian	Brooks
LICHEM	Cisneros
Parallel-in-Time	Maday
Automated Parameterization	Ren; Ho

(3) Development Going Forward (Part A)

(A) Software

Tinker Codes as an Open Platform for Developers
Support for Current Versions of Existing Models (Amber, CHARMM, OPLS, *etc*.)
Support for New and Emerging Force Fields, esp. Polarizable Methods
Algorithmics & new Mathematics / Physics
Biophysics, of course, but also "general chemistry", materials, *etc*.

(B) Hardware

CPUs, GPUs, Intel Phi, and others (?)
GPUs: NVIDIA *vs*. AMD, CUDA *vs*. OpenCL
Programming Models: MPI 3.x, OpenMP 4.x

Hybrid CPU / GPU Code
Multi-Platform Support

- ***Thursday, March 16th*** **(17:00-21:00)**

(Whittemore House, 6440 Forsyth Boulevard, 17:00-21:00)

(4) Demonstrations, Code Discussion & Social Hour(s)

We will reconvene at the Whittemore House (*aka*, the Washington University Faculty Club). From 17:00 to 19:00 there will be snacks and an open bar. We will have several computer workstations (iMacs, and a Mac Pro with GTX 980 GPU) set up and connected to the campus network. We will have working versions of the Tinker, Tinker-HP and Tinker-OpenMM codes for testing, benchmark timings, code inspection, *etc*. If you have other software you would like to demonstrate, show or compare, please send them ahead of time, bring them on your own laptop, or be prepared to run things remotely from your home machines.

This will hopefully be lots of fun. And since almost everyone at the meeting is a programmer, it will give us a chance to interact in a way that is impossible at traditional meetings. So come prepared to show off your latest efforts by running a test case or example, and be prepared to let others look at your implementation. And we will attempt to answer an age-old question: How many hor d'oeuvres can a room full of developers eat?

From 19:00-21:00, we will have the conference dinner in the Whittemore House dining room. All food and drink expenses for the Social Hour and Dinner will be covered by the Conference. The dinner menu is as follows:

Salad: Whittemore House Salad (Mixed Greens, Spiced Pecans and Walnuts, Red Onion,Cherry Tomatoes, Celery Seed Vinaigrette Dressing)

Entrée: Choice of Either: (1) Missouri Trout with Lemon Hollandaise, and Sun Choke Hash with Sculpted Carrots, or (2) Roasted Chicken Breast with Sweet Sherry Wine Pan Gravy, Ozark Mushroom Risotto and Steamed Asparagus

Dessert: Mixed Berry Tart with Raspberry Sauce

● *Friday, March 17th*

(Danforth University Center, Room 276, 8:30-11:30;
& Danforth University Center, Room 234, 13:00-16:00)

(5) Development Going Forward (Part B)

- TINKER as the reference code; put new methods / code there first, and then move to TINKER-HP, OpenMM, etc.
- Integration of the three Tinker code bases (merge at "TINKER 9" ?)
- Multiple versions of polarizable electrostatics, or a single version – ??
  - Tinker 8, Tinker-HP, QI; Speed Comparisons
  - Refactoring to enable MPI
  - Refactoring to enable Domain Decomposition
- Tests of importance of dispersion PME (?)
- GPUs- What is the Future Path ?
  - Stay in sync with "Canonical" OpenMM
  - Tinker-OpenMM branch with periodic merges
  - Develop new GPU code (CPU/GPU hybrid, AMD, Intel Phi)
- Free Energy Methods and Sampling
  - Alchemical Perturbation (extensions of existing code)
  - Thermodynamic Integration / Metadynamics
  - Lambda Derivatives, *d*U / *d*lambda
  - Soft-Core Electrostatics
  - Updated OSRW Versions
- Double Precision (CPUs) *vs*. Mixed / Single Precision (GPUs)
  - Does it matter? for which Problems?
    - PCG and TCG *vs*. DIIS on GPUs
    - Free Energy Calculations
    - QM/MM (LIChem, CHARMM, Q-Chem, others)
- Trajectory Storage, Transport and Archiving
  - Binary file format(s)
  - Compatibility with ptraj / Amber

(6) Target Application Areas

- Free Energy Simulations
  - FEP, BAR, MBAR, ΔH / ΔS
- QM / MM
- pKa Calculations

Protein & Nucleic Acid Folding
Small Molecule Crystal Simulations
Heavy Metal Ions
Testbed for Polarizable Potentials (Drude Oscillator, *etc*.)

● *Friday, March 17th*

(Gamlin Whiskey House, 236 North Euclid Avenue, 18:00-21:00)

For dinner, we will converge on this restaurant in the Central West End (CWE) neighborhood of St. Louis city, near the Washington University Medical School campus. The location is about a 10 minute walk from the CWE MetroLink station, and we will go there as a group via MetroLink following the afternoon session. Gamlin's is perhaps best known for steaks, but also features a wide variety of modern American entrees. The menu is at http://gamlinwhiskeyhouse.com/. Each attendee will need to pay for their drinks and meal.

● *Saturday, March 18th*

(Bauer Hall, Room 330, "Active Learning Lab", 8:30-11:30)

(7) GitHub / WebSites & License Issues

TinkerTools.org Site
- Documentation
- Regression Testing
- Tutorials
- Classroom & Laboratory Exercises
- Wiki and /or User Forum for Questions

GitHub Site for each Tinker Code
- Version N-1 will be Publically Available
- Public GitHubs will allow Free Download (including Dompanies)
- Private GitHubs with access for Developers

Proprietary License for now; between Washington Univ., Univ. Texas-Austin snd UPMC / Sorbonne

(8) Organization of Software Development

Hierarchy of 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 8 & Tinker-HP Papers
Submitted, with Core Developers as authors

Tinker 9 Publication
Possibly "Merged" Code; More Authors including Developers

Tinker "Reference"
Cite Individual Papers *vs*. all-inclusive “Website” Reference

● *List of Attendees*

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