

Tinker Software Workshop 2019

Sorbonne Université, July 21-22, 2019

All meetings are at Laboratoire Jacques Louis Lions

(Tower 15-16, 3rd floor, room 309: map on page 2)

• July 21st, Sunday (9:00-12:00 am & 13:30-16:30 pm)

9:00-9:30 Breakfast

9h30-12h30 New models & force fields

Topics: overview of the current status of various models in development and what have been changed since the last meeting: AMOEBA+/Hippo/SIBFA/Bond Capacity Model/EVB

Sehr Naseem Kahn (UNT)

Sameer Varma (USF)

Roseane Silva (WashU)

Daniele Loco (SU)

Louis Lagardère (SU)

Brandon Walker (UT Austin)

Francis Jing (UT Austin)

12:30-14:00 Lunch

14:00-15:30 Sampling & statistical mechanics methods

Topics: overview of the current advances in sampling.

Mark Tuckerman (NYU)

Frédéric Célerse (SU)

Discussions about integrators/OSRW/Virial-barostats code/Path Integrals etc...

15h30-16h00 Coffee break

16:00-18:00 Code Bases & Programming Models (Ponder)

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

1. Tinker: Ponder
2. Tinker-HP: Piquemal
3. Tinker-OpenMM: Ren
4. OpenMM: Eastman
5. PMEMD-GEM (Amber): Cisneros
6. CHARMM: Brooks
7. FFX: Schnieders

19:30 Tinker diner (Atelier Maître Albert, 1 rue Maître Albert 75005 Paris)

<https://www.ateliermaitrealbert.com/>

July 22nd, Monday (9:00-12:00 am & 13:30-16:30 pm)

9:00-9:30: Breakfast

9:30-10h30: Code evolutions

Topics: overview of the current code developments: CPUS/vectorization/GPUs/new platform/visualization

Vectorization (Tinker-HP): Luc-Henri Jolly (SU)

Visualization, VTX Demonstration: Maxime Maria (Limoges)

11:00-11:30: Gaussian QM/MM interface, Filippo Lipparini, Pisa (Skype Talk)

11:30-12:30: GPUs discussion

Double Precision (CPUs) vs. Mixed / Single Precision (GPUs) Does it matter? for which Problems?

12:30-14:00: Lunch

14:00 Algorithms & Methodology

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

New algorithms from Leuven (J. Harvey)

New algorithms from Paris Saclay (C. Clavaguéra)

15:00-17h00: Discussion about future directions and licences

Access to Sorbonne Université : métro Jussieu (line 7)

