Tinker Software Workshop 2019

Sorbonne Université, July 21-22, 2019

All meetings are in Laboratoire Jacques Louis Lions

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

● 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

Speakers:

Sehr Naseem Kahn (UNT)

Sameer Varma (USF)

Roseane Silva (WashU)

Daniele Loco (SU)

Louis Lagardère (SU)

12:30-14:00 Lunch

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

Topics: overview of the current advances in sampling.

Mark Tuckerman (NYU)

Frederic Célerse (SU)

15h30-16h00 Coffee break

16:00-18:00 Code Bases & Programming Models (Ponder)
(Approximately 10 minutes presentation per topic, plus discussion)

Topics: 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 22snd, 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
Visualization, VTX Demonstration: Maxime Maria

11:00-11:30: Gaussian 2020 QM/MM interface, Filippo Lipparini (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
Algorithms from Leuven (J. Harvey)

15:00-17h00: Discussion about future directions

Access to Sorbonne Université : métro Jussieu (line 7)