# CHARMM-TINKER Meeting, Institut Pasteur

# July 18,19,20,21, 2019

## Thursday, July 18

***Continental Breakfast 8:15-9:00***

| **Session I** | **9:00-10:30** |
|---|---|
| William Swope | Polarizable approaches for QM/MM simulations |
| Qiang Cui | Update on QM/MM and coarse-grained models |
| Francesco Paesani | Modeling Hydration, One Molecule at a Time |
| Kwangho Nam | Update of semi-empirical QM/MM methods in CHARMM |
| Jiali Gao | Active-site heterogeneity as illustrated by lactate dehydrogenase |

***Coffee 10:30-11:00***

| **Session II** | **11:00-12:30** |
|---|---|
| Carine Clavaguera | Modeling the IR spectra of ion-containing water |
| H. Lee Woodcock | Accurate QM/MM free energies at affordable costs |
| Jeremy Harvey | Modelling reaction dynamics in solution in Tinker |
| Markus Meuwly | Accurate IR spectroscopy and reactive MD on multiple PESs |
| Arnaud Blondel | Applications of functional transition calculation using POE and SoS |

***Lunch 12:30-2:00***

| **Session III** | **2:00-3:30** |
|---|---|
| Andres Cisneros | GEM and AMOEBA–IL for Classical and QM/MM Methods |
| Milan Hodoscek | Recent Developments in Parallel and QM/MM methods in CHARMM |
| Christian Schroeder | Computing atomic polarizabilities in ground and excited state |
| Michael Crowley | Polymer molecular dynamics: Problems and Successes |
| Michael Feig | Protein structure refinement via molecular dynamics simulations |

***Coffee 3:30-4:00***

| **Session IV** | **4:00-5:30** |
|---|---|
| Themis Lazaridis | Modeling curvature sensitivity in membrane binding |
| Richard Pastor | Membrane Permeability: Part II |
| Wonmuk Hwang | T-cell alpha/beta receptor catch bond dynamics |
| Jianpeng Ma | New results on structural modelling and prediction |
| Fabrice Leclerc | MCSS update with applications |

## Friday, July 19

***Continental Breakfast 8:15-9:00***

**Session I 9:00-10:30**

| | |
|---|---|
| Stefan Boresch | Alchemical free energy simulations without speed-bumps |
| Jay Ponder | Binding free energy calculations with the AMOEBA force field |
| Darrin York | A robust approach for MM->QM free energy Simulations |
| Michael Schneider | GPU-Accelerated AMOEBA thermodynamics |
| Lennart Nilsson | Mutants and α-helical propensity in the Glucocorticoid receptor |

***Coffee 10:30-11:00***

**Session II 11:00-12:30**

| | |
|---|---|
| Charlie Brooks | Free Energy Simulations in Protein Design |
| William Jorgensen | FEP for drug design including of absolute free energies of binding |
| Matthieu Montés | Enhancing the user-interaction with a molecular system: UDock for Tinker |
| Carol Post | Conformational equilibrium of the Src catalytic domain from ABPO |
| Emanuele Paci | Disordered peptides, helical polyampholytes and the role of phosphorylation |

***Lunch 12:30-2:00***

**Session III 2:00-3:30**

| | |
|---|---|
| Ioan Andricioaei | Enhanced, Wind-Assisted Trajectory Sampling |
| Jerome Henin | The Collective Variables module |
| Amedeo Caflisch | Enhanced sampling, Markov state models, and bias removal |
| Sergio Hassan | Self-adaptive multiscaling method for highly crowded media |
| Victor Ovchinnikov | GPU acceleration of multigrid Poisson-Boltzmann electrostatics |

***Coffee 3:30-4:00***

**Session IV 4:00-5:00**

| | |
|---|---|
| David Perahia | Conformational exploration of macromolecules with normal modes |
| Jingzhi Pu | Update on Reaction Path Force Matching |
| Wei Yang | Sampling enhancement of molecular dynamics simulations |
| Daniel Roe | Implementation of the Action-CSA method in CHARMM |
| Jana Shen | A paradigm shift in computer-aided drug discovery for kinase |

## Saturday, July 20

***Continental Breakfast 8:15-9:00***

**Session I 9:00-10:30**

| | |
|---|---|
| Gregory Beran | Reducing computational cost of polarizable force fields |
| Toshiko Ichiye | Biomolecular force fields for the extremes |
| Peter Eastman | The HIPPO force field in OpenMM |
| Alex MacKerell | Status of the additive C36 and polarizable Drude force fields |
| Nohad Gresh | The SIBFA polarizable molecular mechanics/dynamics potential |

***Coffee 10:30-11:00***

**Session II 11:00-12:30**

| | |
|---|---|
| Benoit Roux | Benoit's Jambalaya: polarizable force field, kinase, and ion channels |
| Teresa Head-Gordon | Applications of reduced SCF and SCF-less methods |
| Andrew Simmonett | Particle mesh Ewald theory for modern compute architectures |
| Louis Lagardère | Multiple-timestep strategies for polarizable point dipole MD |
| Thomas Simonson | Drude polarizable force field model for methyl phosphate with Mg2+ |

***Lunch 12:30-2:00***

**Session III 2:00-3:30**

| | |
|---|---|
| Alston Misquitta | Applications of SAPT(DFT) and the ISA and ISA-Pol algorithms |
| Xiongwu Wu | Use of the Homogeneity Condition for Periodic Sum Potentials |
| Jean-Philip Piquemal | Scalable polarizable molecular dynamics using Tinker-HP |
| Pengyu Ren | Improving AMOEBA(+) force field |
| Julia Rice | Development of "consistent" fixed charge force fields |

***Coffee 3:30-4:00***