



JCAD 2019
JOURNÉES CALCUL ET DONNÉES
Rencontres scientifiques et techniques du calcul et des données

Du mercredi 9 au vendredi 11 octobre 2019
Maison de la Recherche et de la Valorisation
Campus de Rangueil - Toulouse

Meeting intensive and diverse computational requirements for chemists: insights from PSMN@Lyon

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10/10/2019 Toulouse



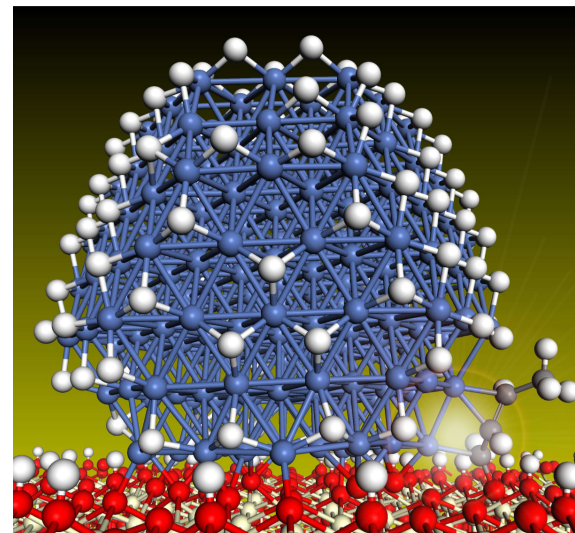
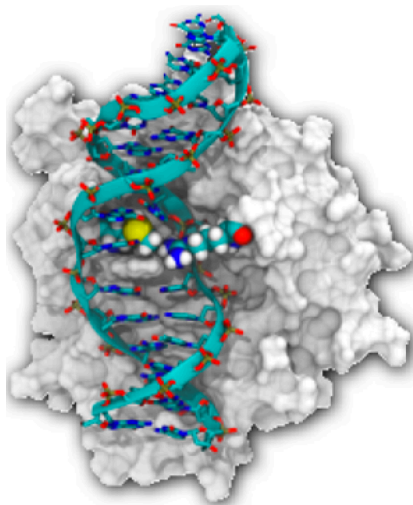
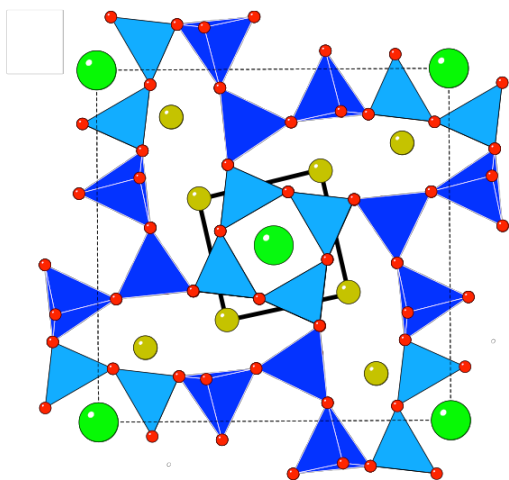
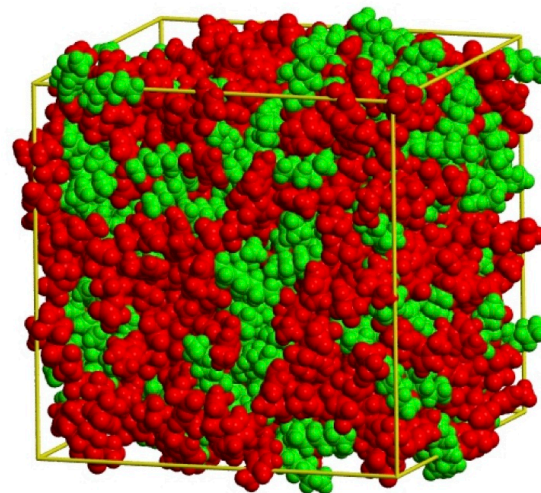
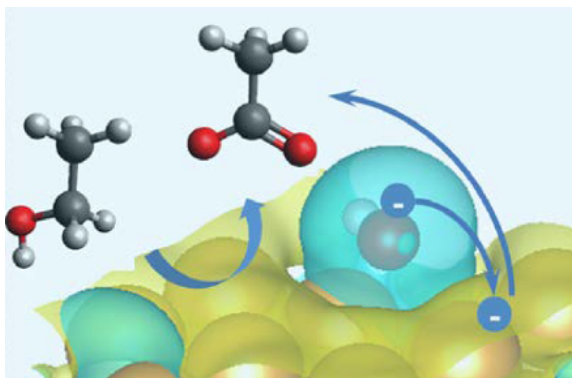
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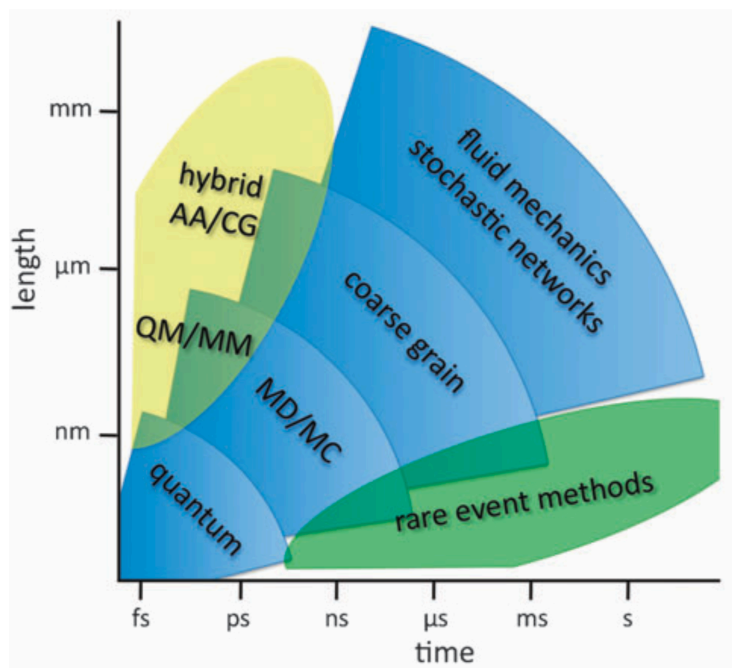
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Chemistry in TC team of LCH



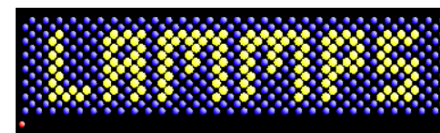
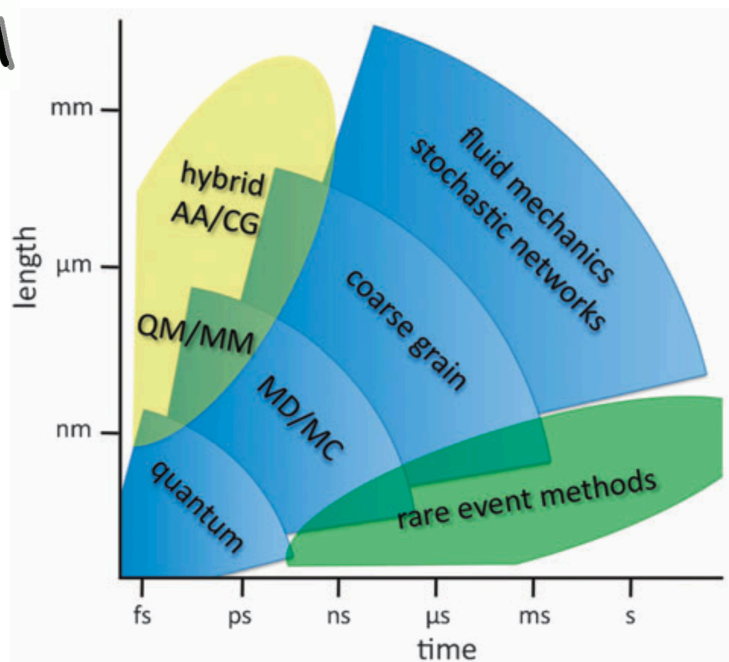
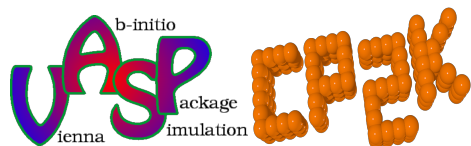
Simulations in chemistry for IT people



method	Type of calculations	Cost	Parallelization overhead
Quantum	Matrix operation	N^3	High
MM	Vector norms	cN	Low
QM/MM	MO / VN	N^3	difficult
Coarse grain	Vector norms	cN/n	Low

Software that we use

FlexMD FDynamic Cobram

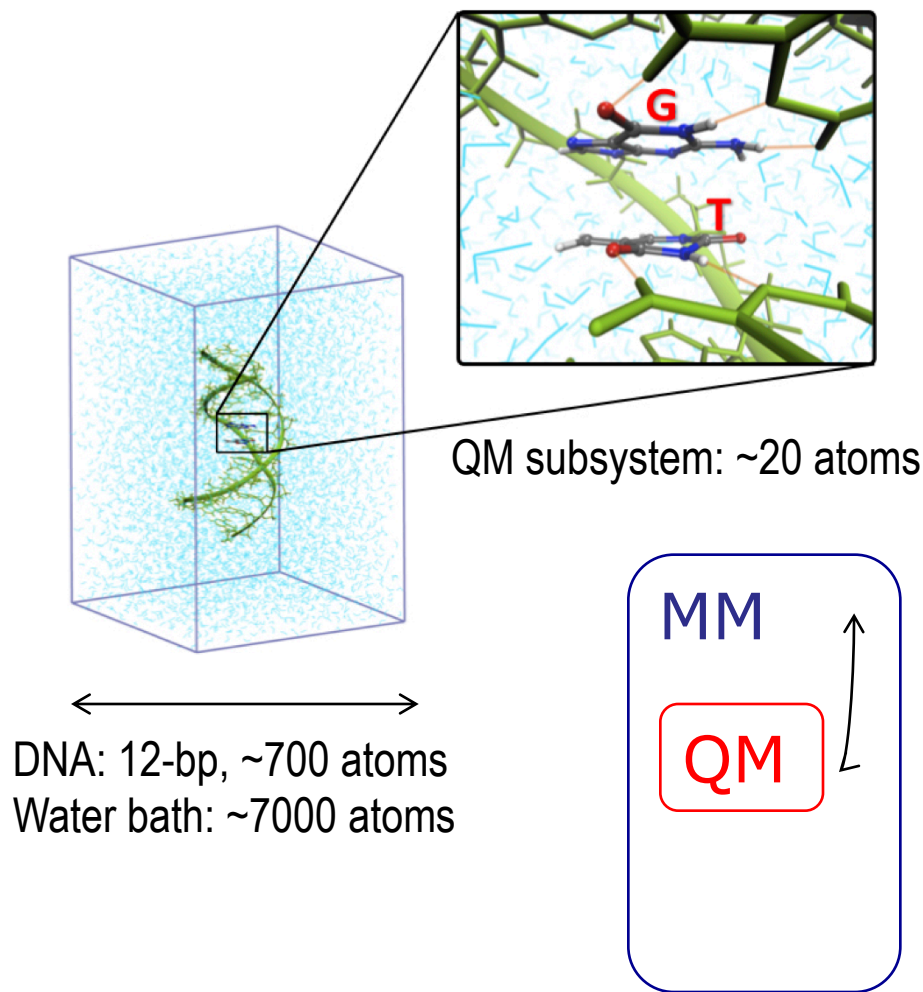


Amber

NAMD
Scalable Molecular Dynamics



Case 1: QM/MM Molecular Dynamics



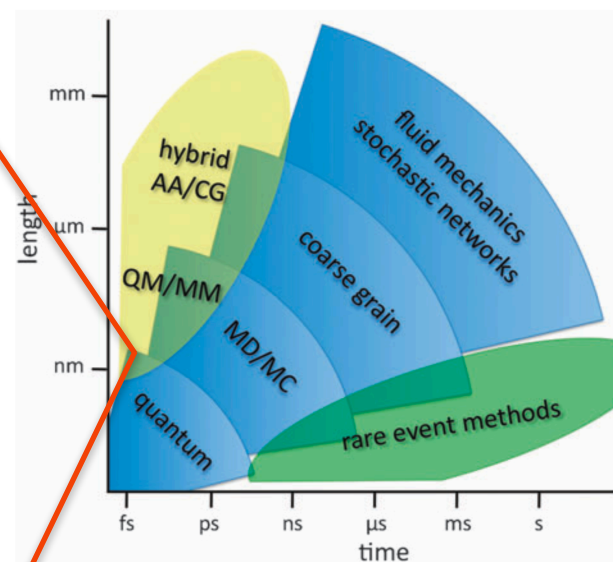
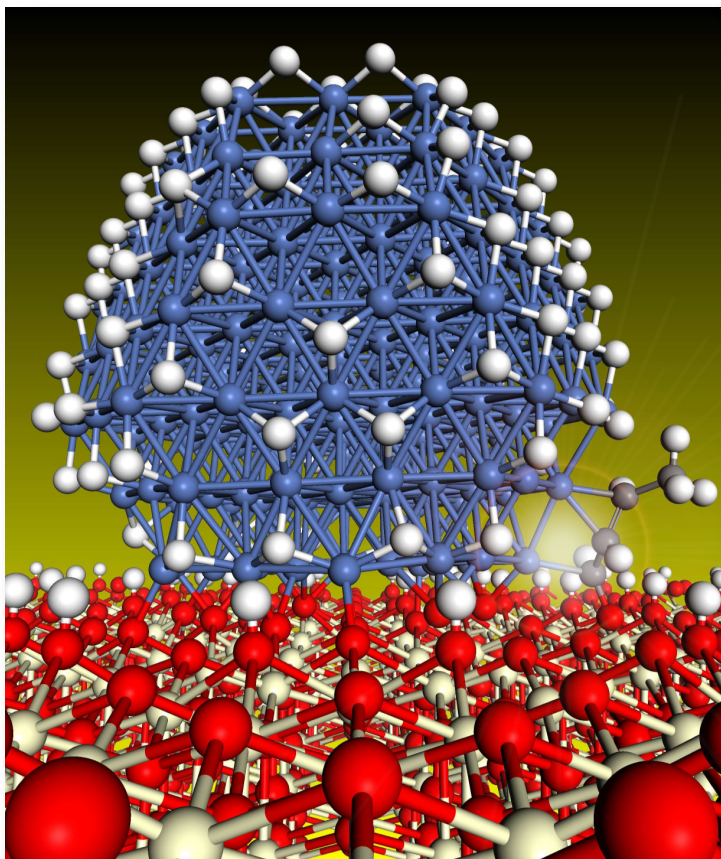
Wrapper around different codes

- Passes data between codes via file handling
- Collect data from codes and give final result

Issues

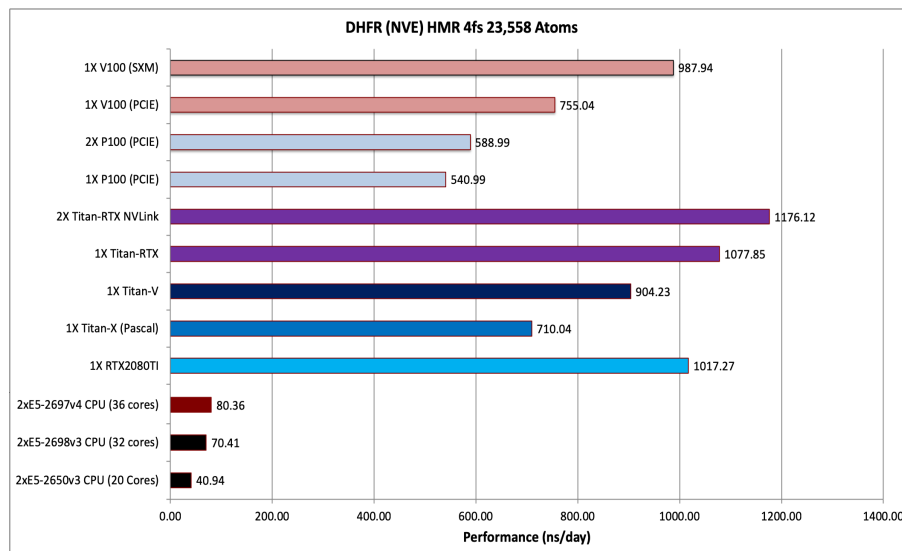
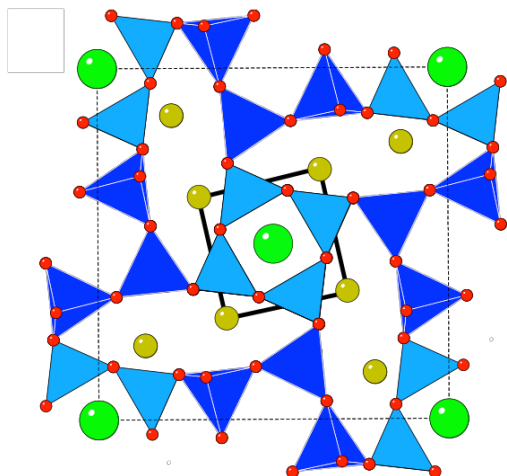
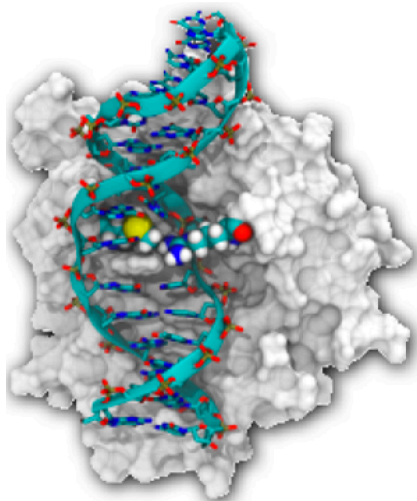
- I/O and initiating calculation at each time step
- Difficult to parallelize

Case 2: Study of Nanoparticles



- Touching the limit of quantum mechanics calculation (DFT)
- Doesn't scale well (2 nodes)
- Large files to store and transfer
- Requires days to get check point, hence long walltime required

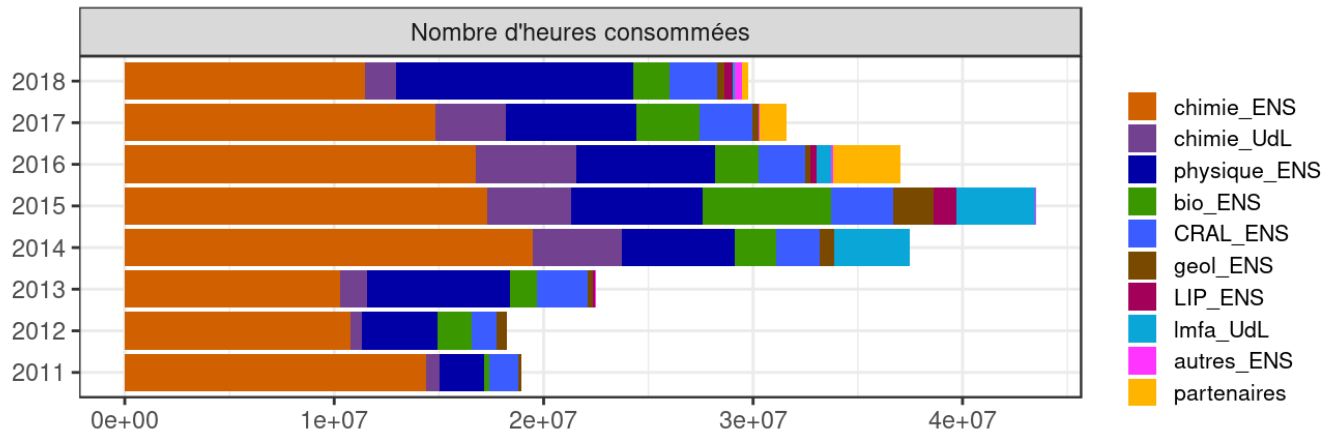
Case 3: Special hardware



- Special equipment (GPU, SSD)
- Large memory (16 GB per core)
- Large files (up to TB per file) to store and transfer

Conclusion

- Provide specific queues for specific calculations
- Close to our storage facility
- Provide machines for special hardware requirement
 - GPU
 - SSD
 - RAM
- Test facility before production on National centers



Acknowledgement

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- ENS de Lyon