Quantum Monte Carlo simulations for Alzheimer's disease on the Curie machine :

Efficient strategies for extreme parallelism on petascale platforms and beyond

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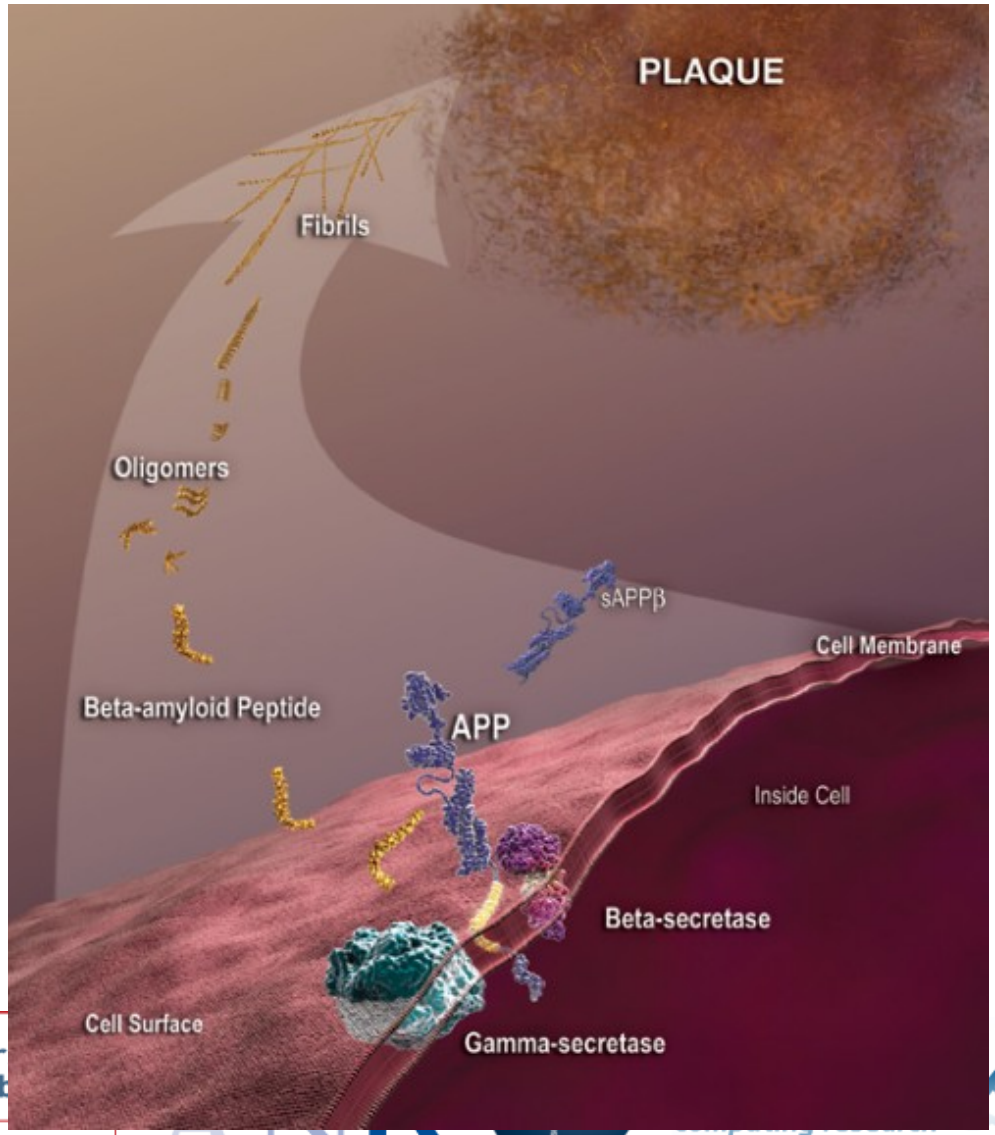
Amyloid plaques agregation

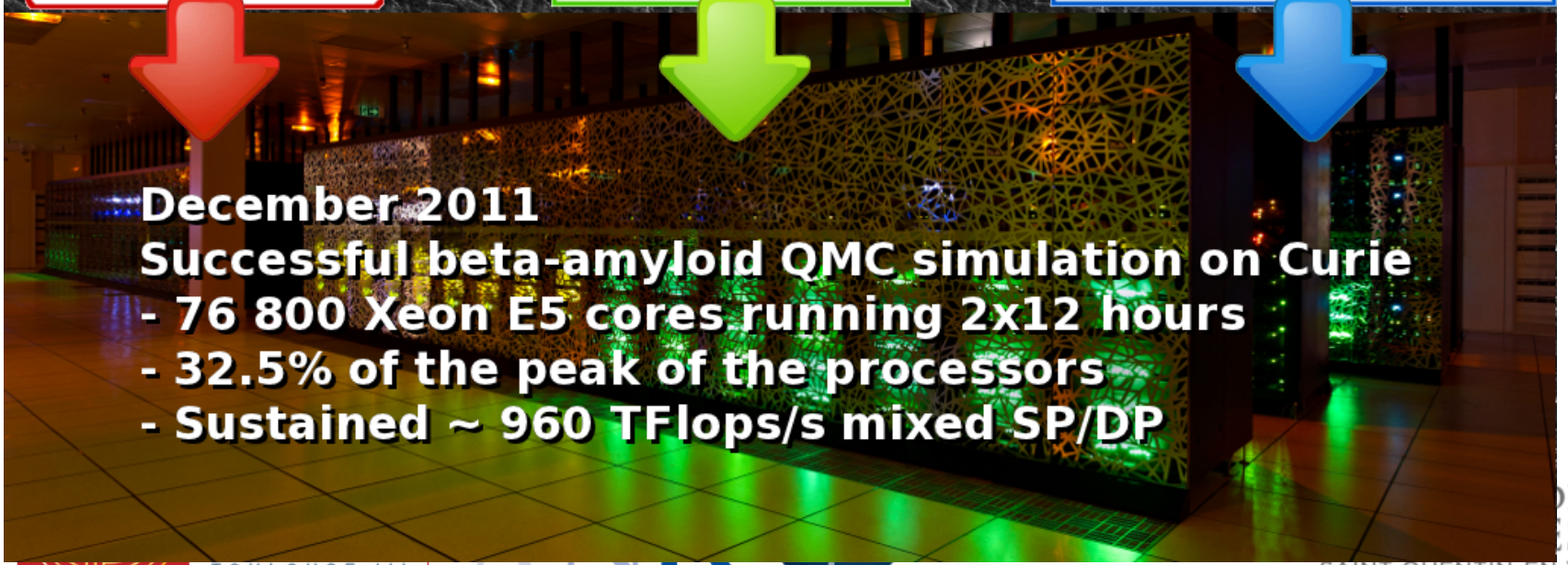


Partners

M. Caffarel, A. Scemama
* QMC Methods
* QMC=Chem code

GENCI: Leader of national HPC resources
* Provides Curie

W. Jalby, E. Oseret
* Performance analysis tools
* Xeon E5 optimization



December 2011
Successful beta-amyloid QMC simulation on Curie
- 76 800 Xeon E5 cores running 2x12 hours
- 32.5% of the peak of the processors
- Sustained ~ 960 TFlops/s mixed SP/DP

Quantum Monte Carlo for molecular systems

Problem : Solve stochastically the Schrödinger equation for N electrons in a molecule

$$
\begin{aligned}
E &= \frac{\int \mathrm{d}\mathbf{r}_1 \ldots \mathrm{d}\mathbf{r}_N \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \mathcal{H} \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)}{\int \mathrm{d}\mathbf{r}_1 \ldots \mathrm{d}\mathbf{r}_N \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \Phi(\mathbf{r}_1, \ldots, \mathbf{r}_N)} \\
&\sim \sum \frac{\mathcal{H}\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)}{\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)}, \text{ sampled with } (\Psi \times \Phi)
\end{aligned}
$$

$\mathcal{H}$: Hamiltonian operator

E : Energy

$\mathbf{r}_1, \ldots, \mathbf{r}_N$: Electron coordinates

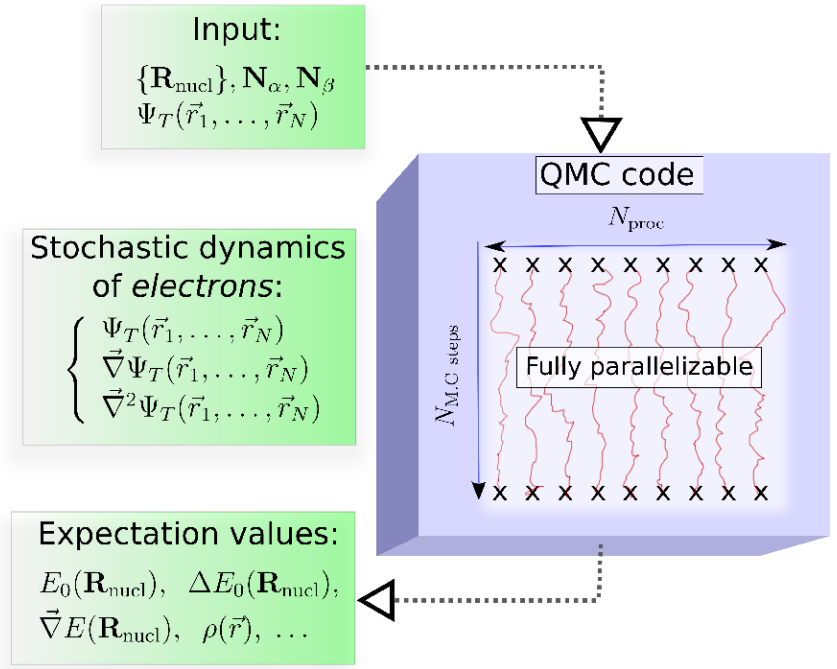
Φ : Exact wave function

Ψ : Trial wave function

QMC Algorithm

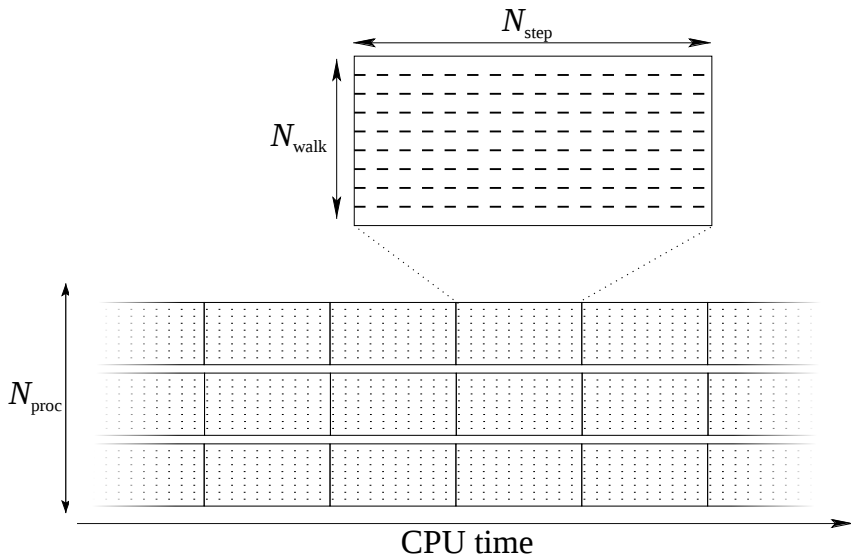
- Walker : vector of $\mathbb{R}^{3N}$ containing the electron positions
- Drifted diffusion of walkers with birth/death process to generate the $3N$-density $(\Psi \times \Phi)$ (needs Ψ, $\nabla\Psi$, $\Delta\Psi$)

- Compute $\frac{\mathcal{H}\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)}{\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)}$ for all positions
- The energy is the average of all computed $\frac{\mathcal{H}\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)}{\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)}$
- Well suited to extreme parallelism : Independent populations of walkers can be distributed on different CPUs

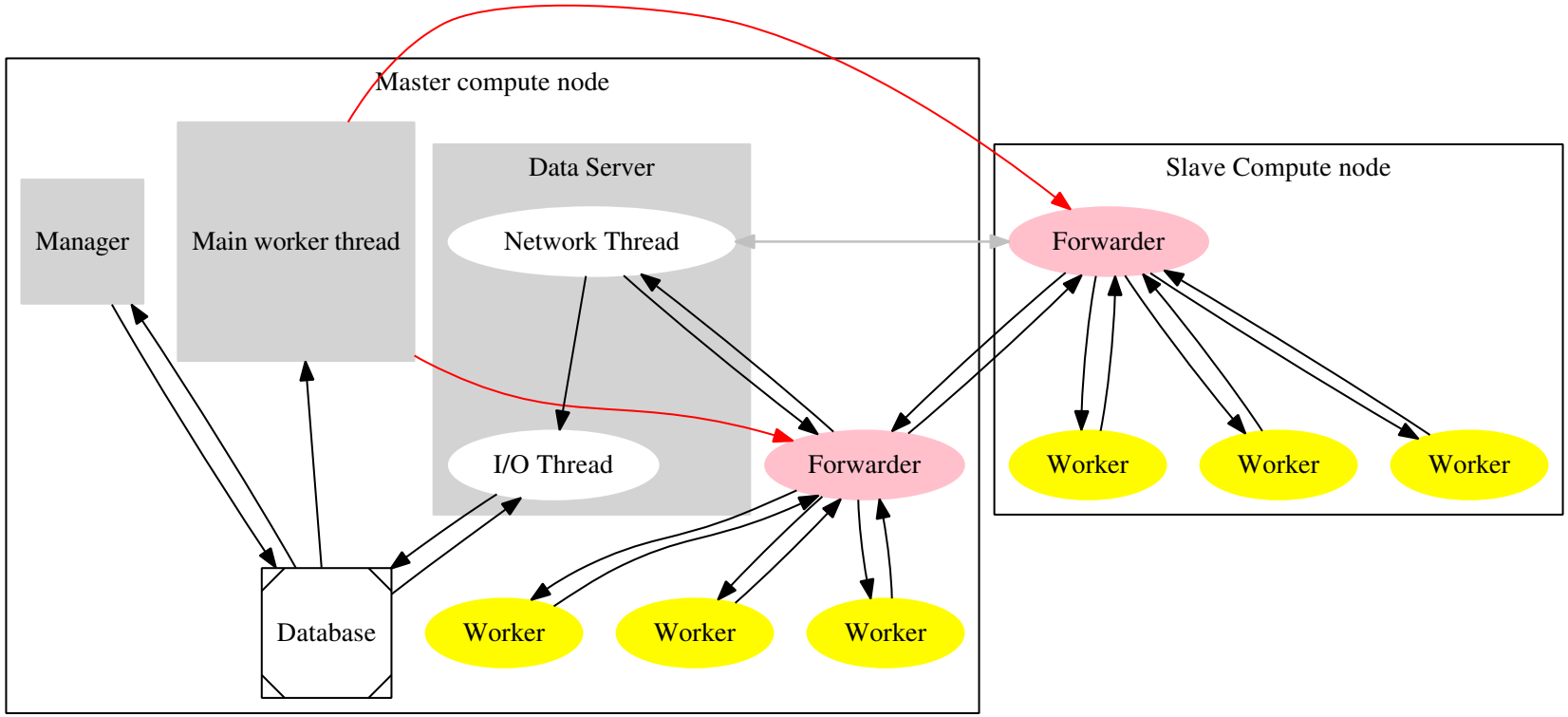


Implementation in QMC=Chem

- Compute as many blocks as possible, as quickly as possible
- Block averages have a Gaussian distribution

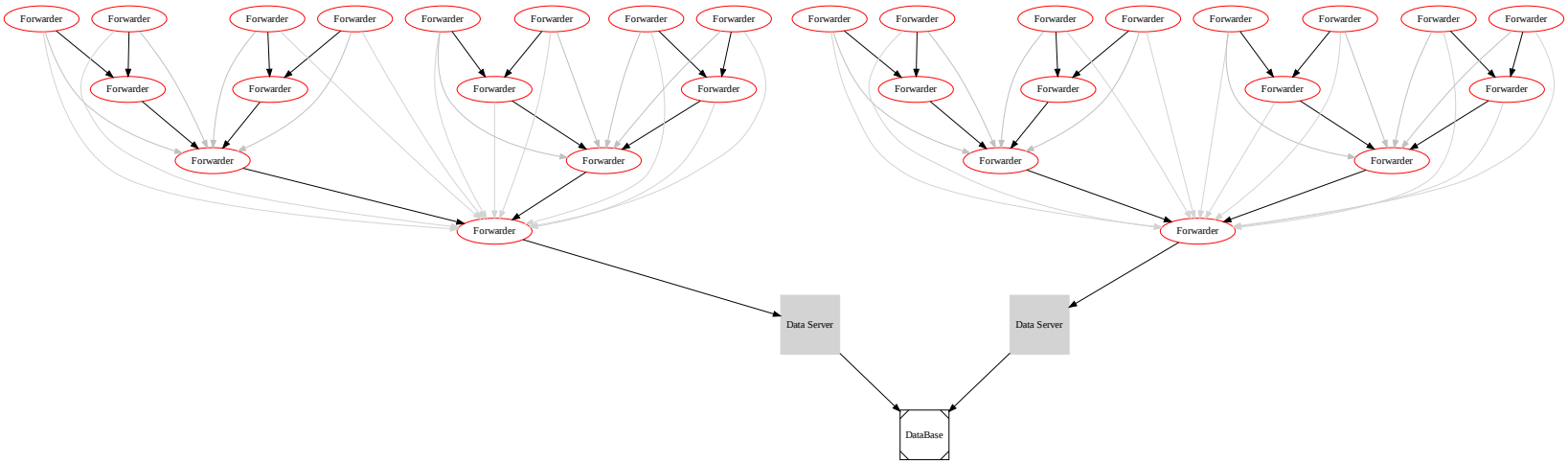


Implementation in QMC=Chem



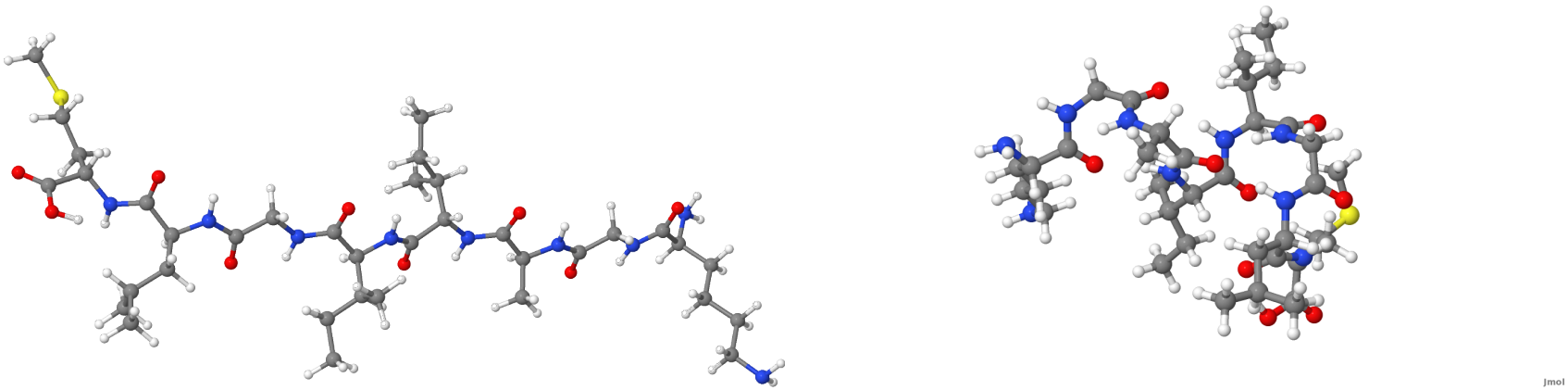
Fault-tolerance

- Blocks are Gaussian $\rightarrow$ losing blocks doesn't change the average
- Simulation survives to removal of any node
- Restart always possible from data base



Amyloid β peptide simulation on Curie

All-electron calculation of the energy difference between the β-strand and the α-helix conformations of amyloid peptide Aβ(28-35)



122 atoms, 434 electrons, cc-pVTZ basis set (2960 basis functions)

Amyloid β peptide simulation on Curie

Scientific results (cc-pVTZ basis set) :

- Standard DFT (B3LYP) : 10.7 kcal/mol
- DFT with empirical corrections (SSB-D) : 35.8 kcal/mol
- All-electron MP2 : 39.3 kcal/mol
- QMC : 39.7 $\pm$ 2. kcal/mol

Technological results :

- Sustained 960 TFlops/s (Mixed SP/DP) on 76 800 cores of Curie
- $\sim$ 80% parallel speed-up. (Today, it would be > 95 % : run termination was optimized)