Massively-Parallel Real-Time TDDFT Modules for Non-Equilibrium Electron Dynamics

NSF: SI2-SSE project

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Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) Simulations

$$\left\{ i\hbar \frac{d}{dt} \left| \phi_i(t) \right\rangle = \hat{H}_{KS} \left| \phi_i(t) \right\rangle \right\}_{i=1..N} \qquad \hat{H}_{KS} \equiv -\frac{\hbar^2}{2m_e}\nabla^2 + \hat{V}_{ext}(t) + \hat{V}_H[\{\phi_i(t)\}] + \hat{V}_{XC}[\{\phi_i(t)\}]$$

Coupled non-linear PDEs w/ millions of PWs for representing the single-particle states.

$$\phi_i(\mathbf{r},t) = \psi_{n\mathbf{k}}(\mathbf{r},t) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}}^{\mathbf{G}_{max}} C_n(\mathbf{G},\mathbf{k},t) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$$

Challenges addressed through development of new modules in Qb@ll code

Highly scalable numerical integrators

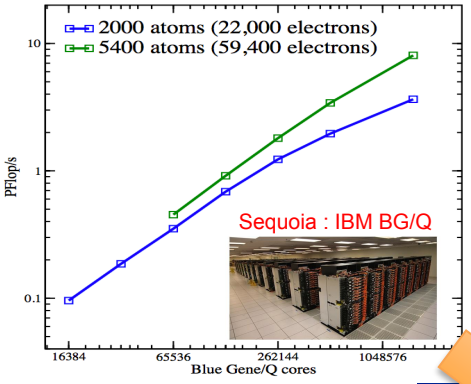
Various integrator methods are made available by interfacing the Qb@ll code with the PETSc library, to reduce "time-to-solution".

Advanced and efficient approximation to V_{xc}

Recent XC functionals such as *Strongly Constrained and Approximately Normed (SCAN)* approximation are implemented in the context of PW-based RT-TDDFT.

Adaptation to various HPC machines

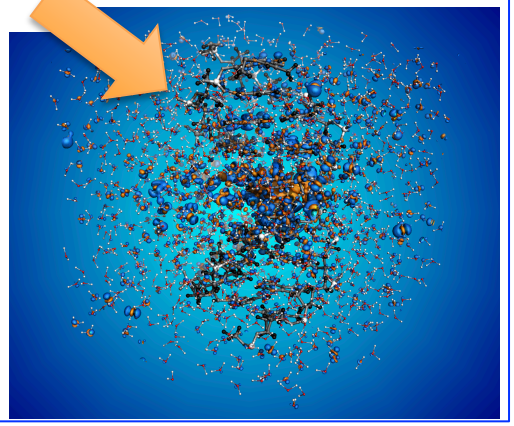
The code is designed to scales over a very large number of cores (>200K) on various HPC architectures, including IBM-BG/Q, Cray Blue Waters, KNL Theta, etc.



HPC Software Infrastructure

>40% peak performance
@ 1.6 million cores

- Massively parallel and tailored to modern HPCs with hybrid MPI/open-MP/SIMD.



Scientific Impacts

Simulating electronic excitation dynamics in solvated DNA under proton irradiation.

> 12,000 electrons
> 6,000,000 PWs
> 131,000 cores on BG/Q