Max Webinar

BigDFT

Concluding Remarks and Outlook

Luigi Genovese

Laboratoire de Simulation Atomistique - L_Sim

November 12, 2020

Virtual Room

Large Scale DFT. Why?

Motivations behind BigDFT code — Since 2008

- Test the potential advantages of a new formalism
- ☛ A lot of outcomes and interesting results
- Future opportunities and ideas

A code used in production since 2008

A new formalism: Opens the path towards new opportunities
We built the code to perform novel, disruptive approaches

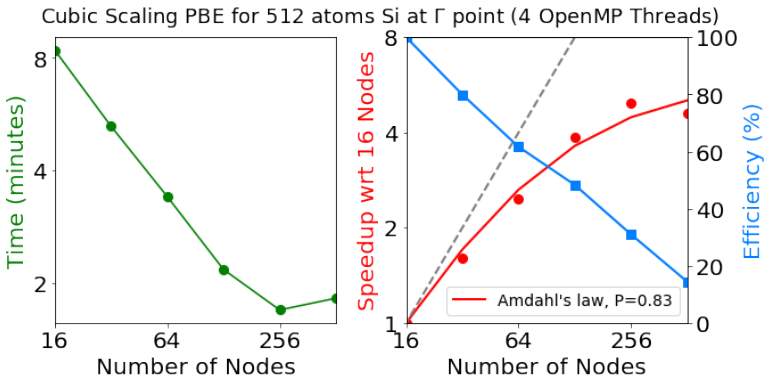
Why Do We Need QM for Large Systems?

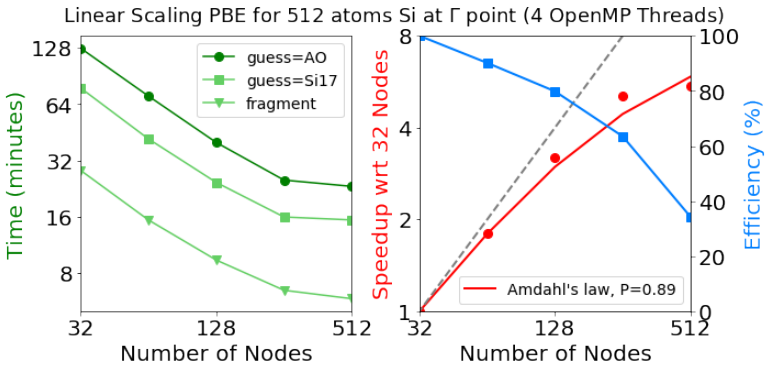
- new possibilities for simulating complex materials
- intrinsically QM quantities, e.g. electronic excitations
- Understand information about systems' constituents and the suitable way of modelling their interaction by reducing *a posteriori* the complexity of the simulation

Perspective on Parallel Performance

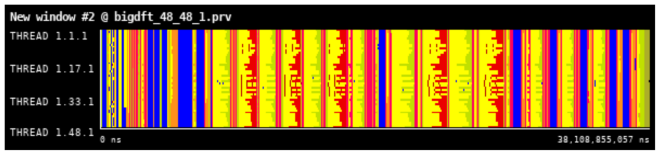
Performance of BigDFT

- good scaling up to $\sim$ few atoms per node
- POP analysis – OpenMP target for improvement
- future analysis – MPI performance at scale





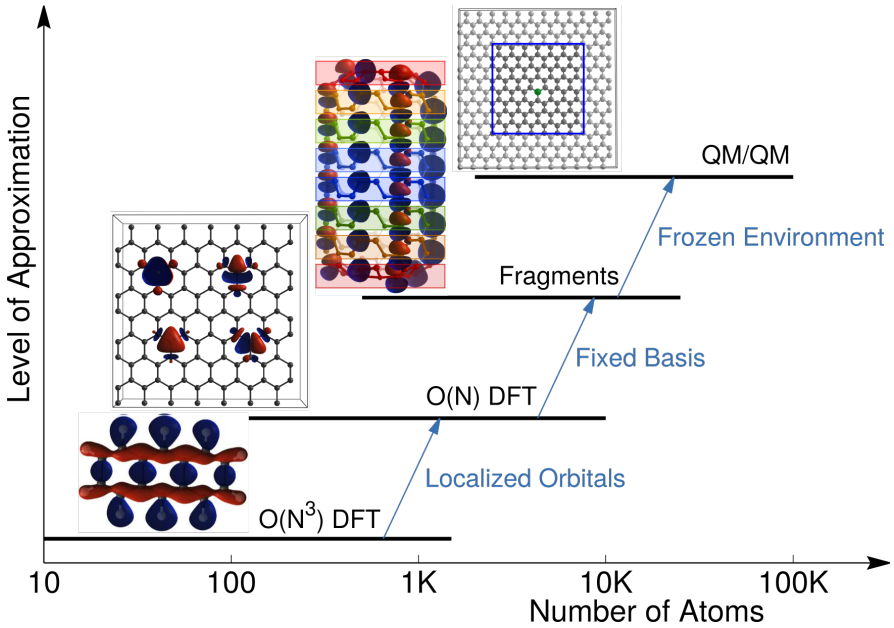
BigDFT Performance Assessment

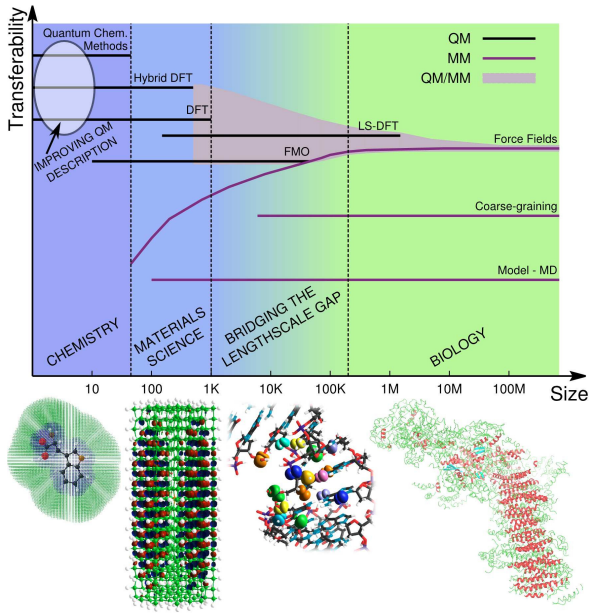


DFT with Wavelets

Across Lengthscales with Wavelets

- three methods in BigDFT with differing levels of approximation
- can go between methods, i.e. fragment $\rightarrow$ linear $\rightarrow$ cubic
- approximations are controllable – can estimate or measure errors





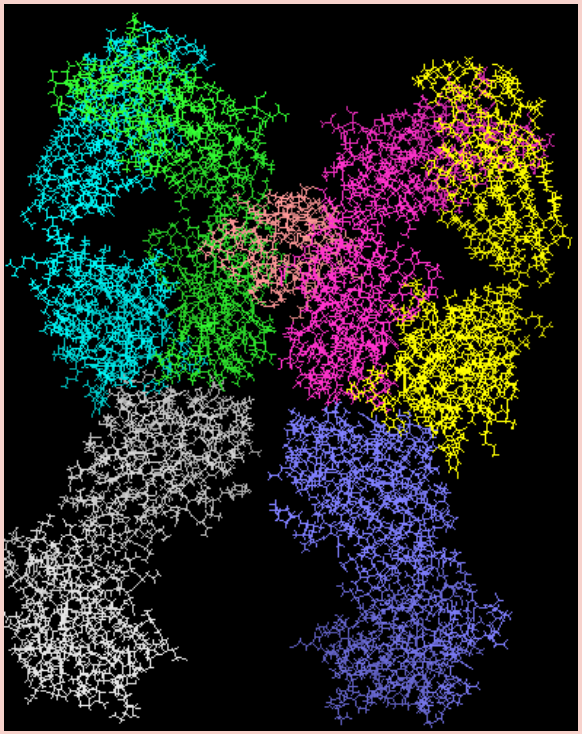
Lots of Systems of interest in Biology

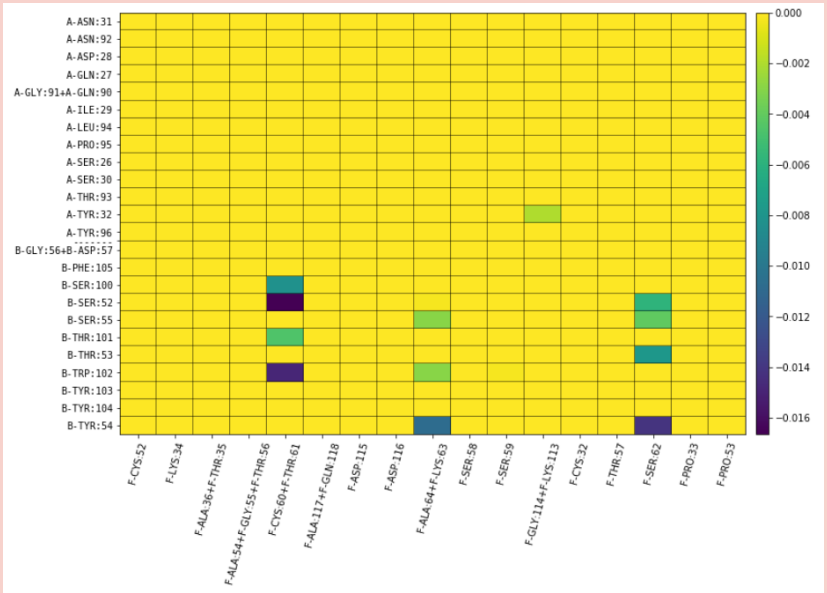
Large systems are routinely accessible

Linear Scaling code $\rightarrow$ CPU time *per atom*

Example: 1400 Residues (One Monoclonal Antibody). 3h of walltime on 32 nodes of IRENE-Rome Machine

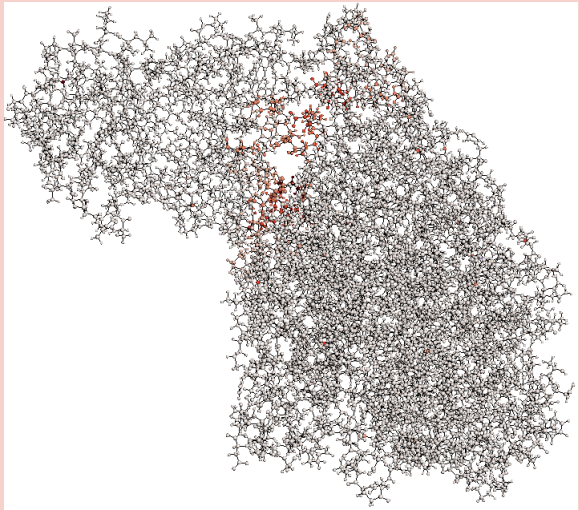
Reduce the number of interactors in a biological system

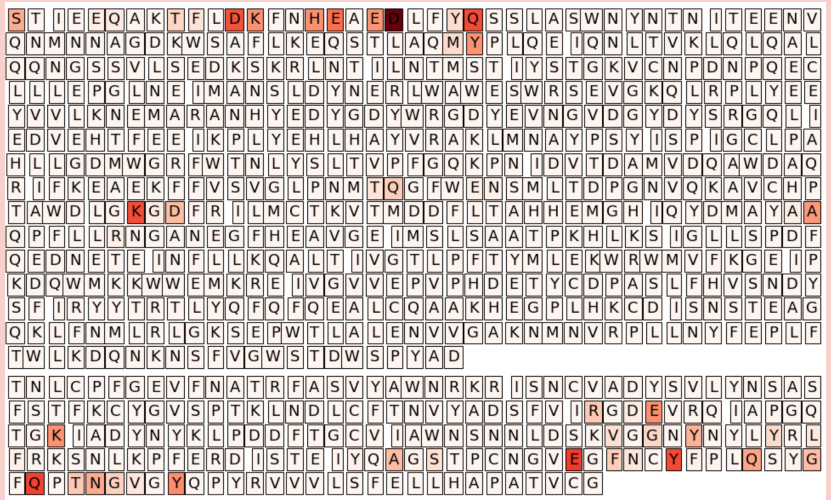




Application to COVID Emergency

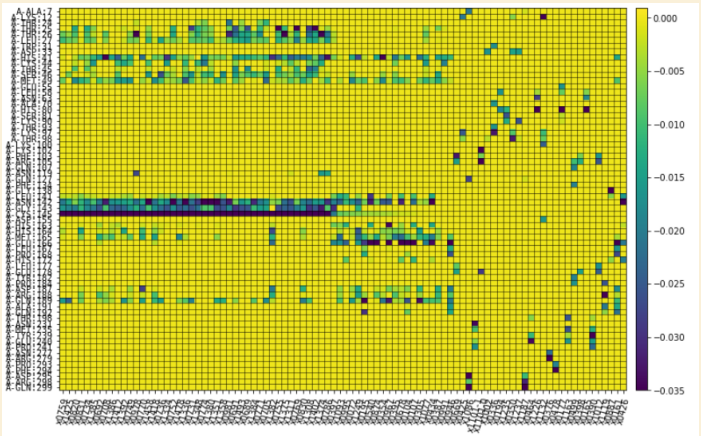
Interactive region of RBD-ACE2 Complex in SARS-CoV-2





COVID Moonshot project

Map the interactions of a dataset of inhibitors from crystallographic positions

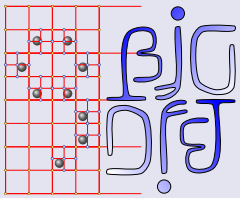


BigDFT Rebranding (coll. w/ NextMol)

Solution become robust

Some algorithmic solution are now ready to be employed for a end-user

New user API, new visual identity



Continuous integration, development model, logo and website are under modification ☛ new user experience

Future scientific directions

Linear-Scaling DFT calculations based on wavelets

- Robust convergence, high accuracy and flexibility (BC)
- Reduction in degrees of freedom $\rightarrow$ large systems
- Different level of descriptions (controlling the precision)
  QM $\supset$ Fragments $\supset$ Atomic charges
- Opens up new possibilities

Challenges and future directions

- Explore interplay environment $\leftrightarrow$ electronic excitations (CDFT, QM/MM, statistics...)
- Provide high quality back end for extraction of information for different communities (Biology, Electro-Chemistry, ...)
- Towards a control of the level of theory (QM/QM)

Acknowledgments

London L. E. Ratcliff, M. Stella

Kobe W. Dawson, T. Nakajima

Basel S. De, S. Goedecker

Barcelona S. Mohr

Grenoble A. Degomme, D. Caliste, T. Deutsch, LG

Boston, ILL M. Zaccaria, M. Reverberi, V. Cristiglio

Rome M. D'Alessandro

Catania G. Fisicaro