

Max Webinar

BigDFT

*Concluding Remarks and Outlook*

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November 12, 2020

Virtual Room

## 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

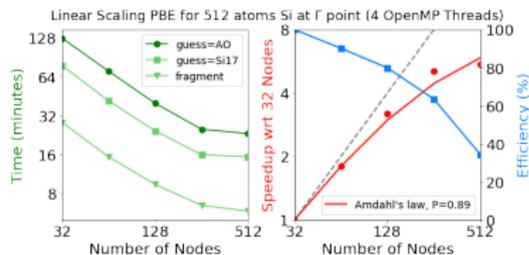
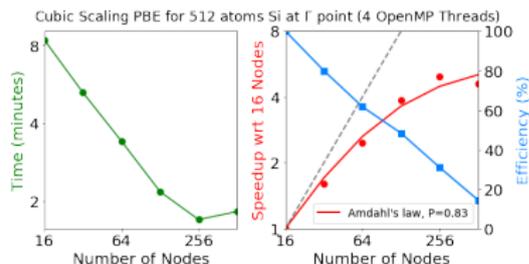
A new formalism: Opens the path towards new opportunities  
We built the code to perform novel, disruptive approaches

## Why Do We Need QM for Large Systems?

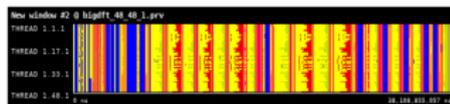
- new possibilities for simulating complex materials
- intrinsically QM quantities, e.g. electronic excitations
- **Understand** information about systems' constituents and the suitable way of modelling their interaction by reducing a *posteriori* the complexity of the simulation

## Performance of BigDFT

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

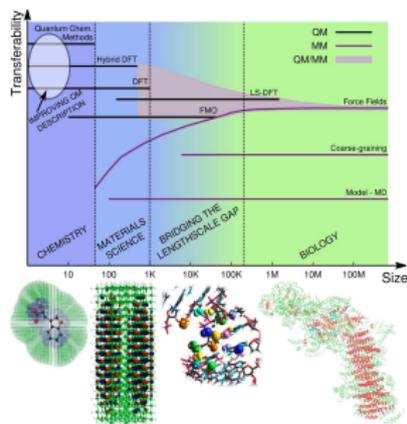
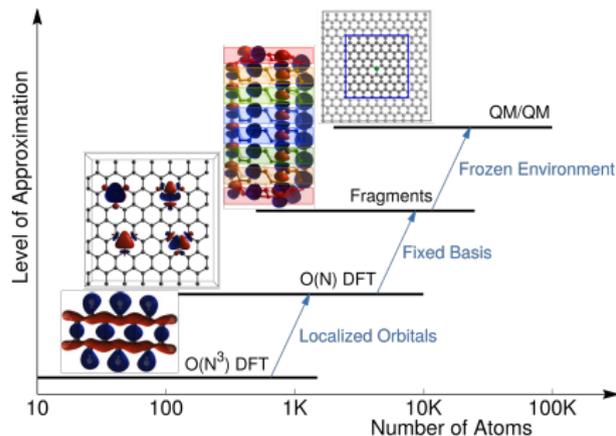


## BigDFT Performance Assessment



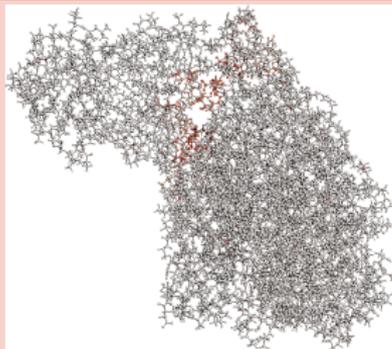
## Across Lengthscales with Wavelets

- 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





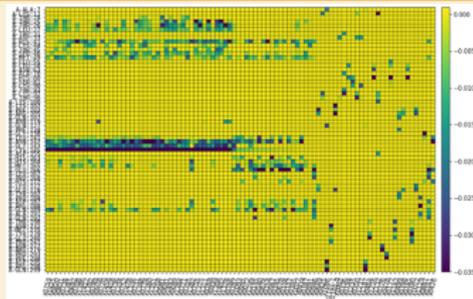
## Interactive region of RBD-ACE2 Complex in SARS-CoV-2



|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
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| Q | N | N | N | A | G | D | K | W | S | A | F | L | K | E | Q | S | T | L | A | O | M | Y | F | L | Q | E | I | Q | N | L | T | V | K | L | Q | L | O | A | L |   |
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| R | I | F | K | E | A | E | K | F | F | V | S | V | G | L | P | N | M | T | O | G | F | W | E | N | S | M | L | T | D | P | G | N | V | Q | K | A | V | C | H | P |
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## COVID Moonshot project

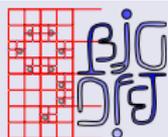
Map the interactions of a dataset of inhibitors from crystallographic positions



## 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



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**A fast, precise and flexible DFT code  
for ab-initio atomistic simulation**

Open source software for innovative research of materials and  
macro-molecular systems at the nanoscale

## 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)

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