Chemistry on Dardel: An opportunity and a challenge

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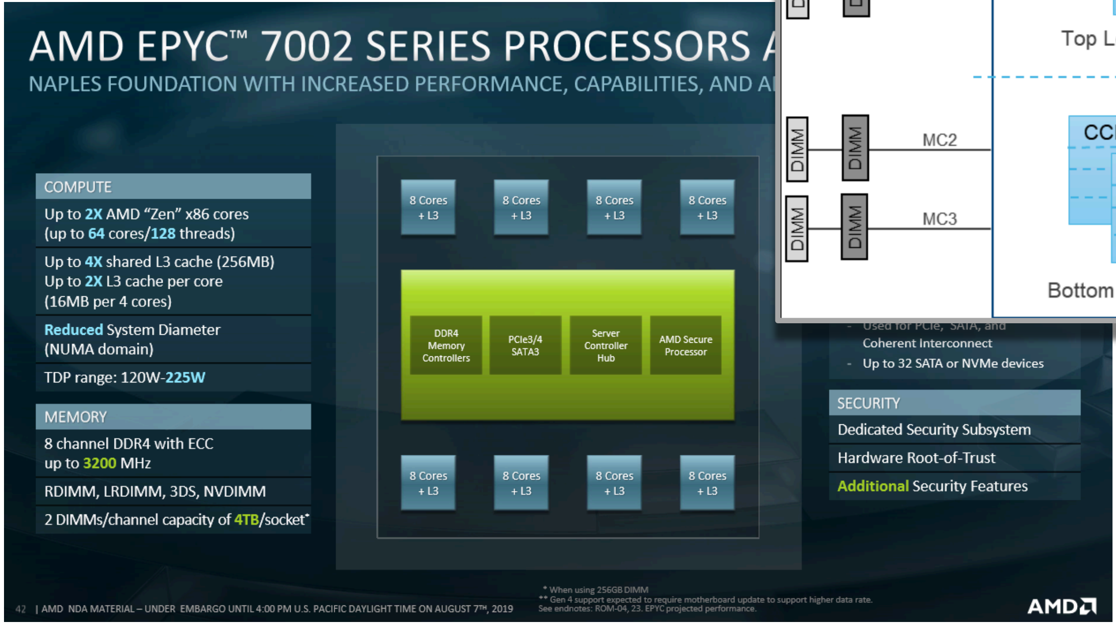
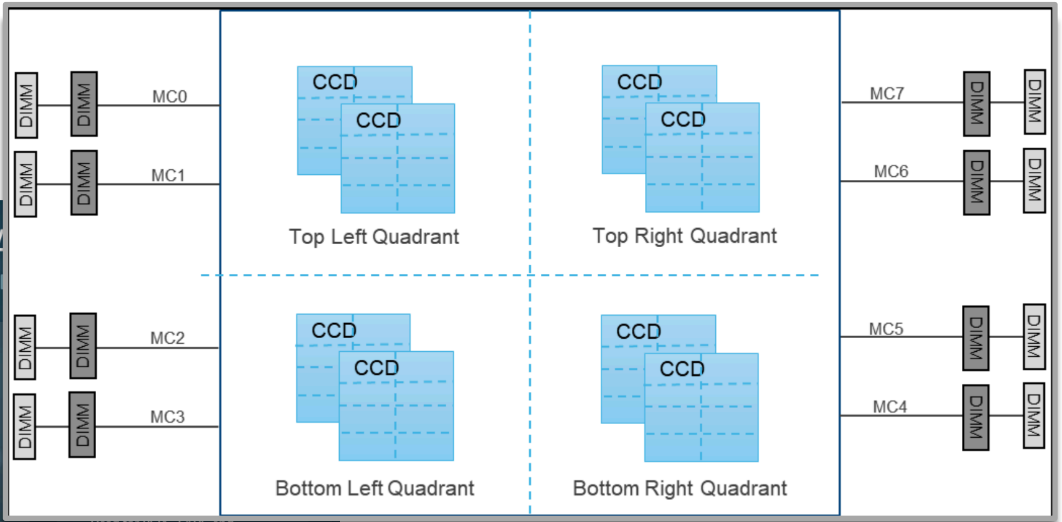
Dardel:
AMD EPYC 7742 64-Core Processor

How can we efficiently perform *in silica* chemistry inside this complex laboratory environment?

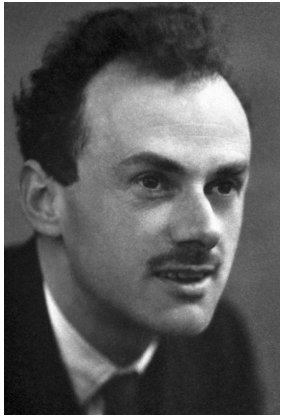




In multi-chip processors like the AMD-EPYC series, differing distances between a CPU core and the memory can cause NonUniform Memory Access (NUMA) issues. – Moham Rockam @ DELL

The fundament is quantum mechanics

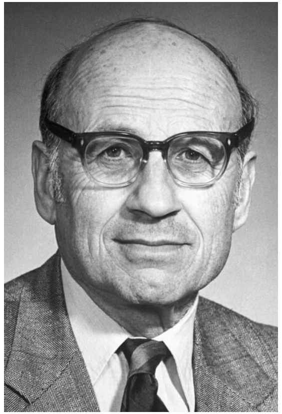
$$\hat{H}\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

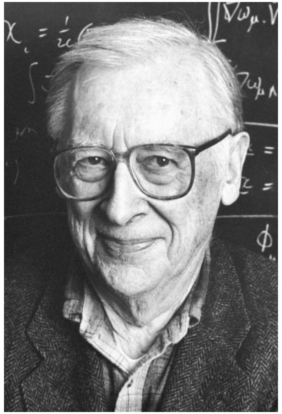


The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of **chemistry** are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.

The Nobel Prize in Physics **1933** was awarded jointly to **Erwin Schrödinger** and **Paul Adrien Maurice Dirac** "for the discovery of new productive forms of atomic theory."

The reason we can do chemistry from first principles



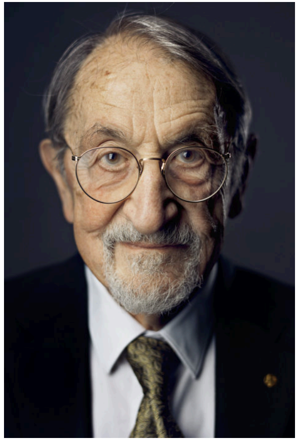


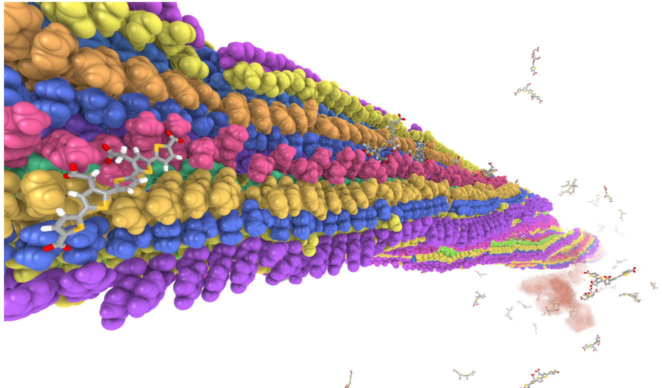
$$\hat{H}\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

$$\hat{f}\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

The Nobel Prize in Chemistry **1998** was divided equally between **Walter Kohn** "for his development of the density-functional theory" and **John A. Pople** "for his development of computational methods in quantum chemistry."

The reason we can treat complex chemical systems





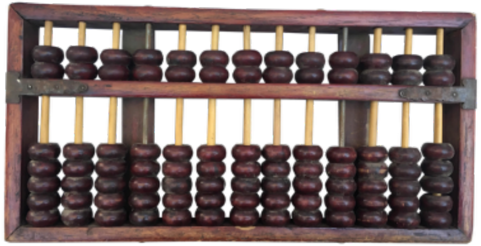
$$\hat{f} \rightarrow \hat{f}^{\mathrm{QM}} + \hat{f}^{\mathrm{QM/MM}} + \hat{f}^{\mathrm{MM}}$$

The Nobel Prize in Chemistry **2013** was awarded jointly to **Martin Karplus**, **Michael Levitt** and **Arieh Warshel** "for the development of multiscale models for complex chemical systems."

Present state of affairs in computational chemistry

1930

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of **chemistry** are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved. — P.A.M. Dirac



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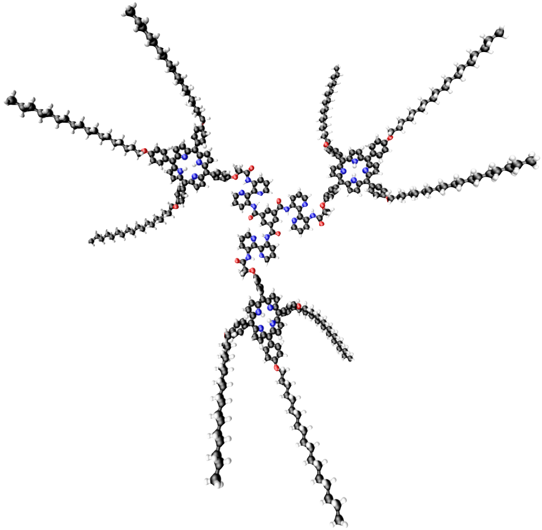
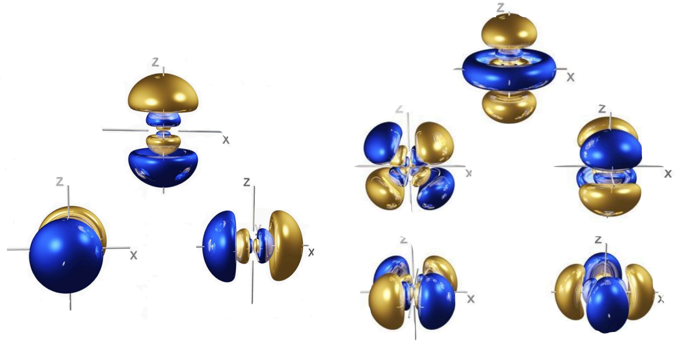
The fundamental methods necessary for the computational treatment of the whole of **chemistry** are thus completely known, and the difficulty lies only in the fact that application of these methods is made prohibitively hard on the all too complex hardware of today.

Turning things into matrix equations by introducing a basis



$$\psi_i(\mathbf{r}) = \sum_{\alpha} c_{\alpha i}\phi_{\alpha}(\mathbf{r})$$



$$\hat{f}\psi_i(\mathbf{r}) = \varepsilon_i\psi_i(\mathbf{r})$$

$$\mathbf{FC} = \mathbf{SC}\boldsymbol{\varepsilon}$$