



Using modeFRONTIER to automate DFT and QMC calculations: applications to liquid hydrogen

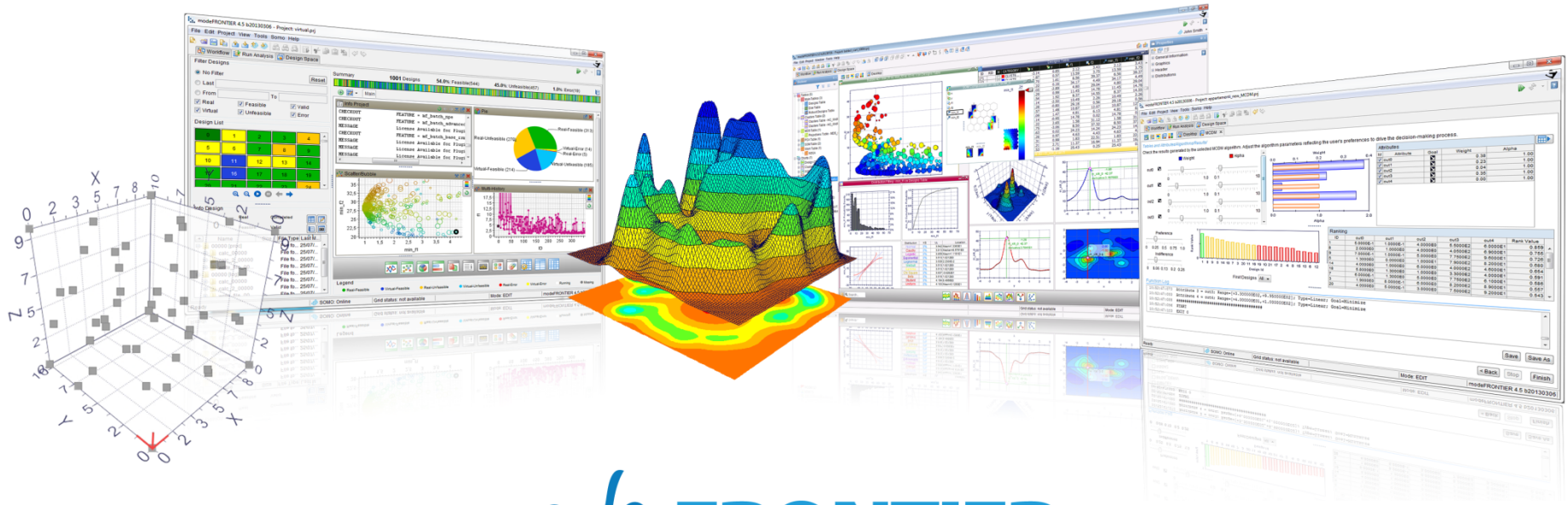
Mariapia Marchi, Danilo Di Stefano (ESTECO S.p.A., Trieste, Italy)

Sandro Sorella, Guglielmo Mazzola, Ye Luo (SISSA)

- Motivation
- Introduction to modeFRONTIER
- Few examples
- Integration of DFT and QMC applied to the study of liquid hydrogen
- Conclusions & Perspectives

From this year QMC conference webpage

A particular topic of interest is the relationship between QMC and density functional theory. In particular, we hope to look towards obtaining a better understanding of the relative benefits of QMC/DFT in systems and situations where DFT often fails, such as in weakly-interacting systems, strongly-correlated materials, metal-insulator transitions, magnetic properties, and biological systems. Furthermore, it is intended to look into the better integration of DFT and QMC codes. In industrial applications, where users typically require ease-of-use and a graphical user interface, how can we move towards a situation where the user may do e.g. pre-screening of candidate structures with the faster DFT, then press a 'Make the Answer Better button' which feeds the relevant wave function files into a QMC programme and spits out reliably accurate energetics for the selected problems. It is also of interest to understand how to 'move the atoms' in QMC i.e. how to exploit the power of QMC in cheaper DFT and classical-force-field molecular dynamics calculations (in the context of 'embedding methods' or otherwise). Additionally we can look at how to use QMC to develop better exchange-correlation functionals for use in DFT. We therefore warmly encourage the participation of DFT people who may never have run a QMC simulation in their lives but are nevertheless interested in the topic. Suggestions for alternative discussion topics and other proposals are welcome.



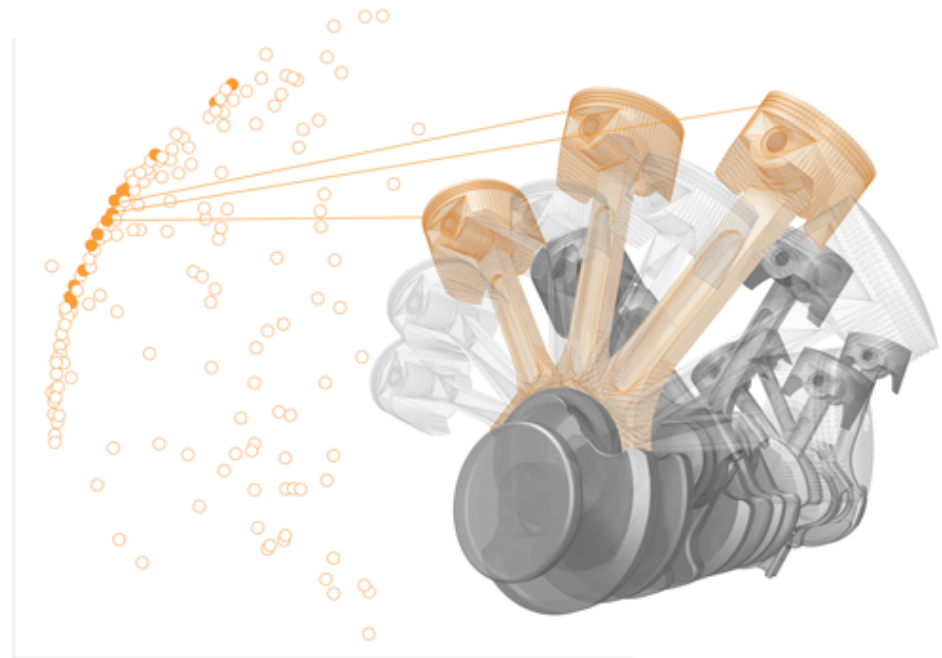
mode FRONTIER

is a commercial software tool. It is an integration platform for multi-objective and multi-disciplinary optimisation. It provides a seamless coupling with third party engineering tools, enables the automation of the design simulation process, and facilitates analytic decision making.

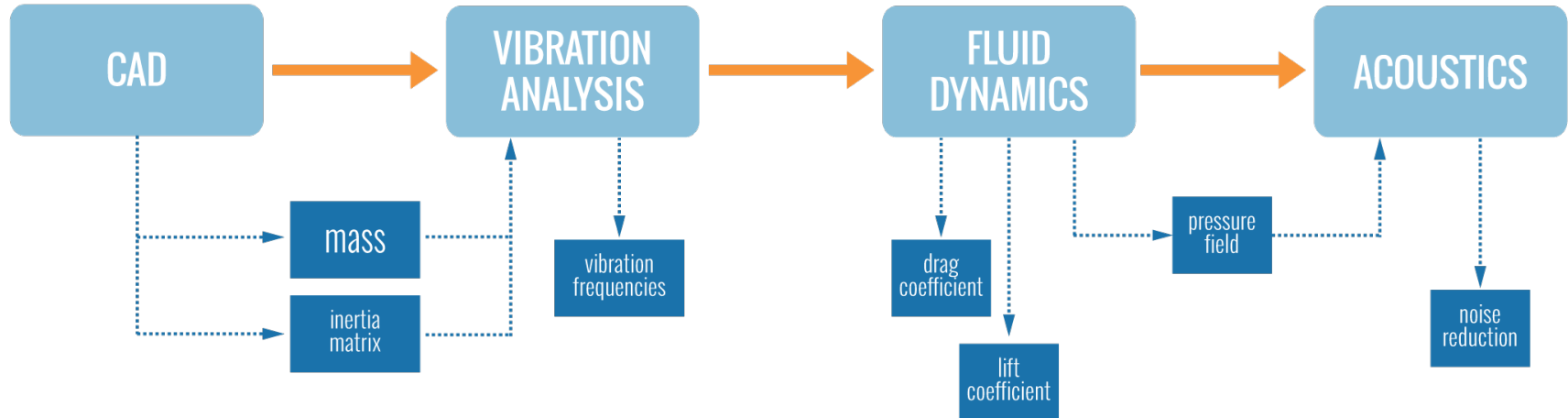
Multi-objective optimisation problems are solved using **optimisation algorithms**, which identify a set of **Pareto designs** for which objective function values are non-dominated by any other design among those tested.

modeFRONTIER allows the user to define the most suitable optimisation strategy according to:

- ✓ number, type and range of variables, objectives and constraints
- ✓ reliability and robustness required
- ✓ attainable computational resources



modeFRONTIER integrates with **any parametric software** (CAD, CAE, FEM, generic, etc.) **automating** the entire optimisation process in which data is transferred from one simulation to the next and the relevant values of outputs and objectives are extracted.

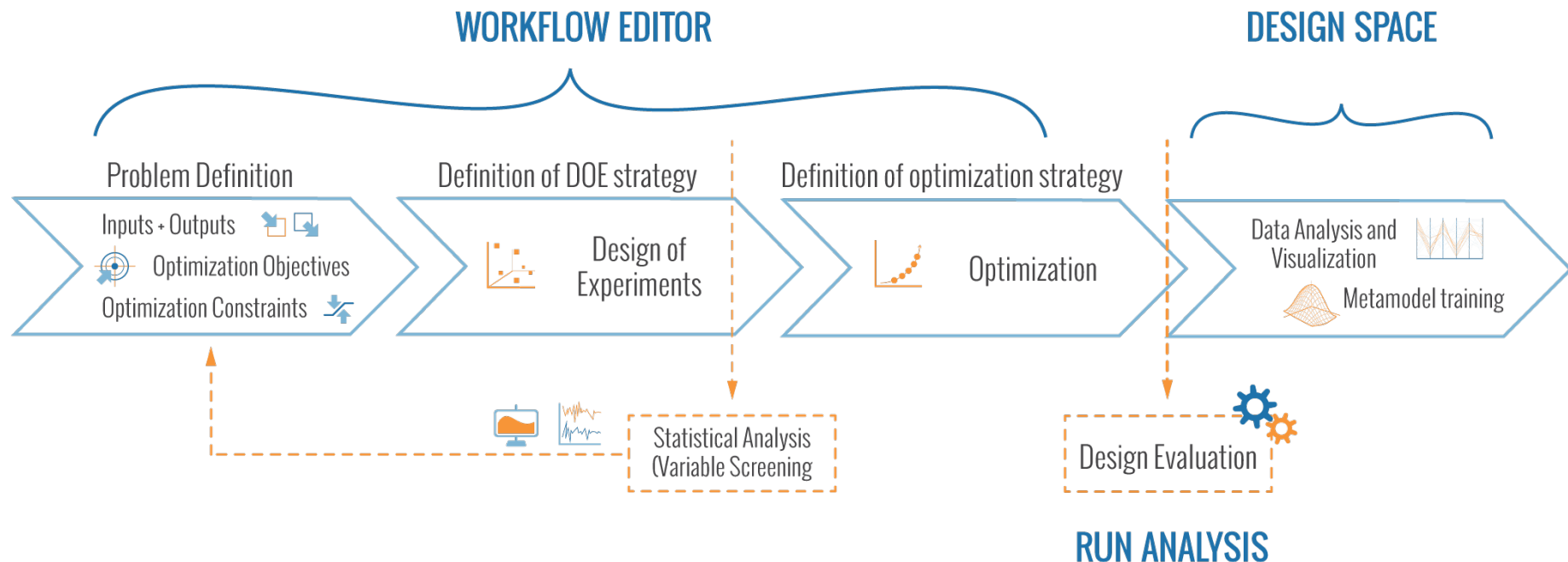


This **multi-disciplinary approach** allows to exploit the **interaction** between the disciplines and determine the **global optimum solution**, instead of optimising each discipline sequentially.

modeFRONTIER is divided in 3 environments,

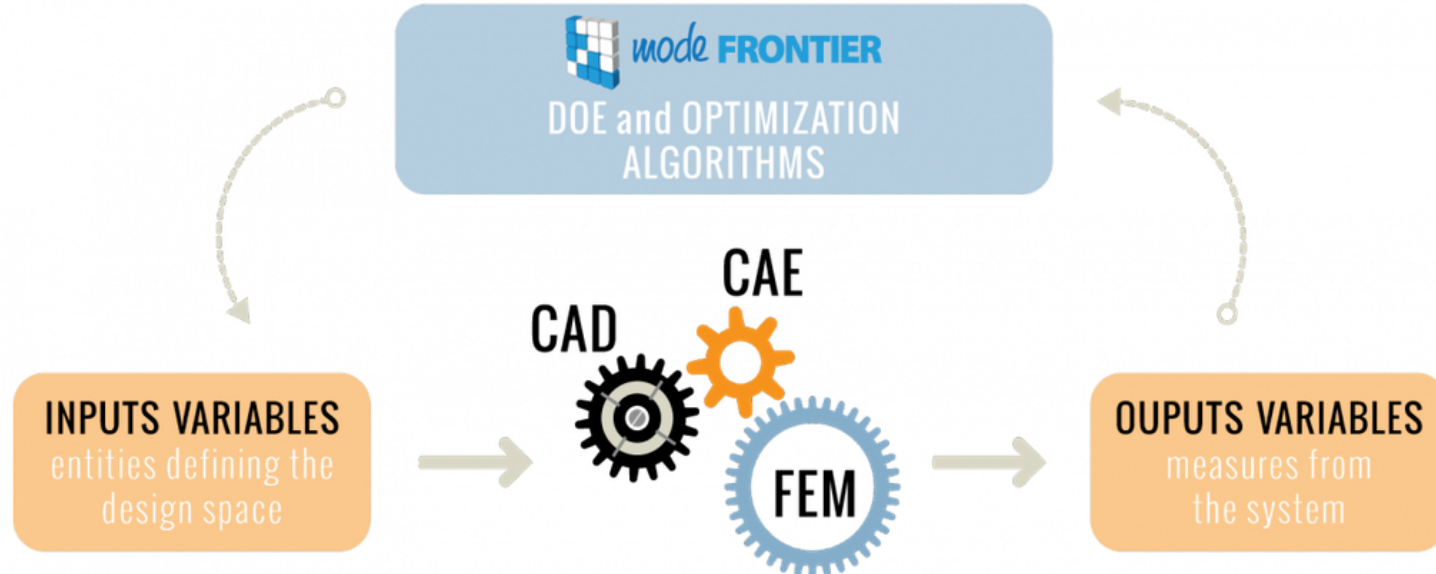
- Workflow
- Run Analysis
- Design Space

each of which is used to accomplish a specific set of tasks tailored to achieve the ultimate goal – **DESIGN OPTIMISATION**.



modeFRONTIER Workflow Editor enables to:

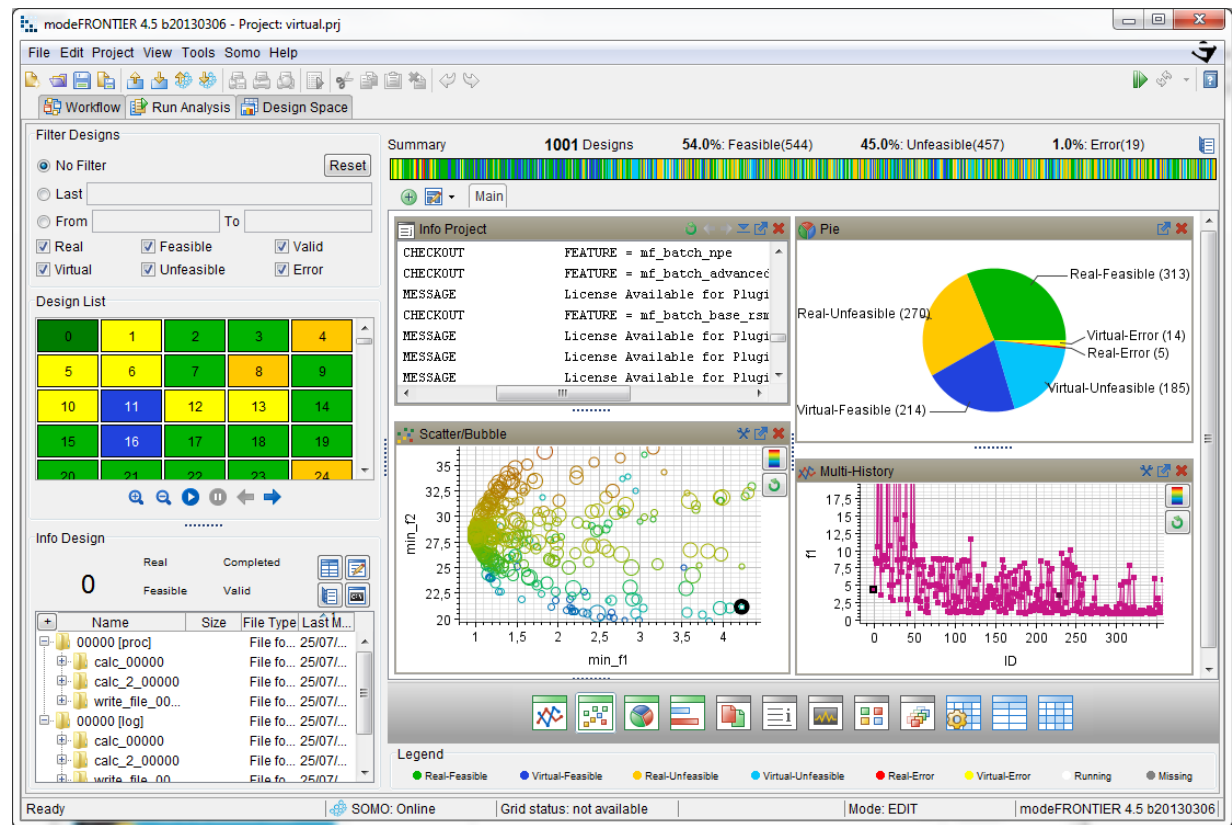
- compose and manage all logical steps of an engineering design problem involving software platforms used in **different disciplines**;
- **automate** the **simulation** process and drive the integrated software platforms, extracting and updating the generated data, and transferring them from one software to another.
- define the I/O variables and **objectives of the optimisation**, and the **DOE and optimisation strategies**



The optimisation "takes place" in the **Run Analysis environment**, enabling real-time monitoring of its progress by means of interactive charts and graphs, and direct access to log and process files.

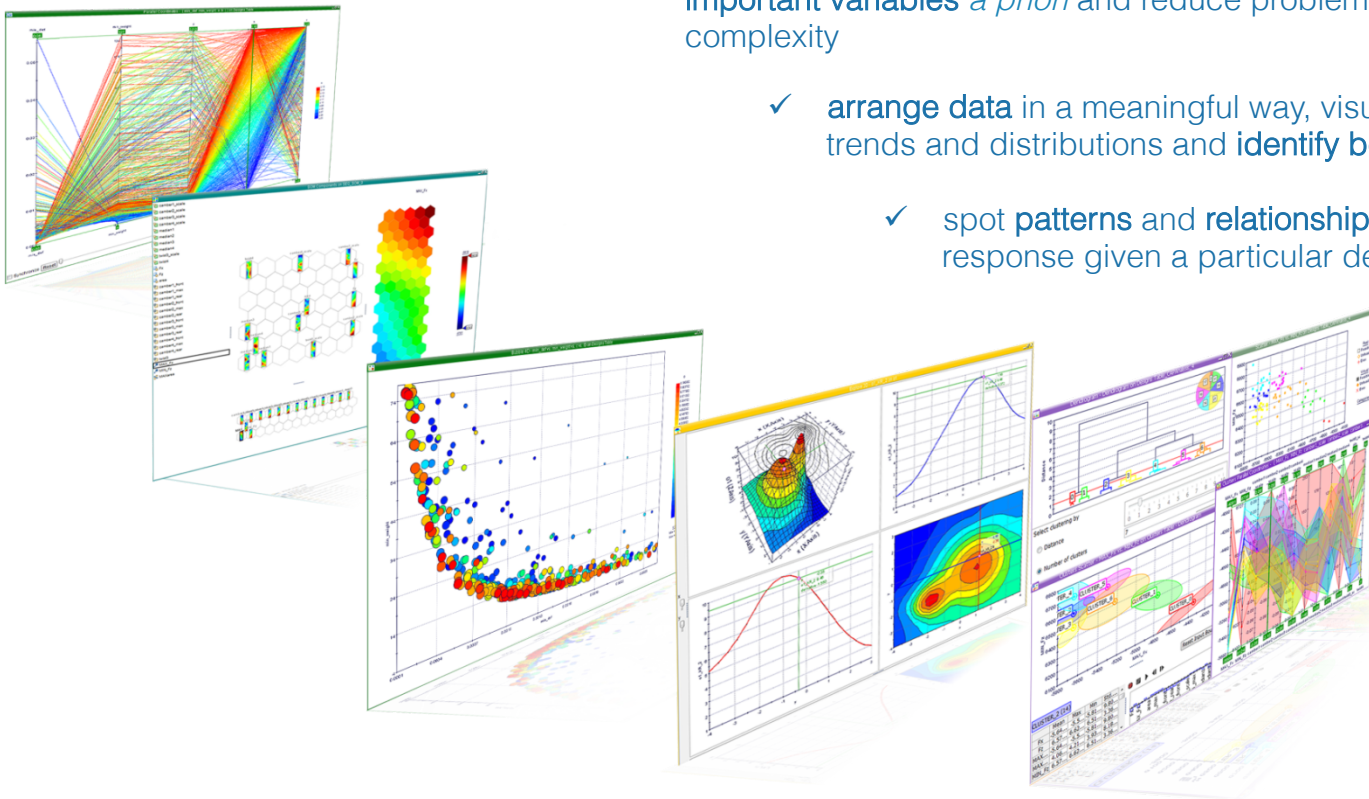
The Run Analysis is:

- entirely **modular** (the dashboard can be customised according to user's preferences)
- dynamic** (as the optimisation advances, all components are automatically updated)



Information underlying the hundreds of complex numerical data generated from parametric studies or optimisation campaigns are collected into tables and can be re-arranged and projected in the charts and graphs of the **Design Space environment** of modeFRONTIER.

- ✓ perform statistical analyses to identify the **most important variables** *a priori* and reduce problem complexity
- ✓ **arrange data** in a meaningful way, visualize optimisation trends and distributions and **identify best designs**
- ✓ spot **patterns** and **relationships** governing the system response given a particular design configuration



IMPROVING FILM DIE FLOW UNIFORMITY USING OPTIMIZATION METHODS COUPLED WITH FINITE ELEMENT CFD ANALYSIS

Patrick C. Lee¹, Laura Dietsche¹, Joseph Dooley¹, Sumeet Parashar²

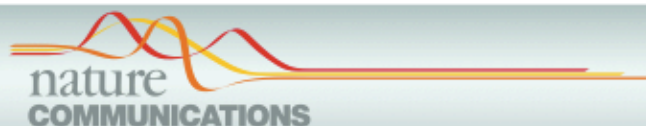
¹The Dow Chemical Company, Midland, MI

²ESTECO North America

DEVELOPMENT AND OPTIMIZATION OF HYDROXYAPATITE – β -TCP FUNCTIONALLY GRADATED BIOMATERIAL

Michael Gasik, Anu Keski-Honkola, Yevgen Bilotsky, Michael Friman*

Aalto University Foundation School of Chemical Technology, P.O.Box 16200, FIN-00076 AALTO



ARTICLE

Received 17 Oct 2013 | Accepted 21 Feb 2014 | Published 19 Mar 2014

DOI: 10.1038/ncomms4487

OPEN

Unexpectedly high pressure for molecular dissociation in liquid hydrogen by electronic simulation

Guglielmo Mazzola^{1,2}, Seiji Yunoki^{3,4,5} & Sandro Sorella^{1,2,3}

The study of the high pressure phase diagram of hydrogen has continued with renewed effort for about one century as it remains a fundamental challenge for experimental and theoretical techniques. Here we employ an efficient molecular dynamics based on the quantum Monte Carlo method, which can describe accurately the electronic correlation and treat a large number of hydrogen atoms, allowing a realistic and reliable prediction of thermodynamic properties. We find that the molecular liquid phase is unexpectedly stable, and the transition towards a fully atomic liquid phase occurs at much higher pressure than previously believed. The old standing problem of low-temperature atomization is, therefore, still far from experimental reach.

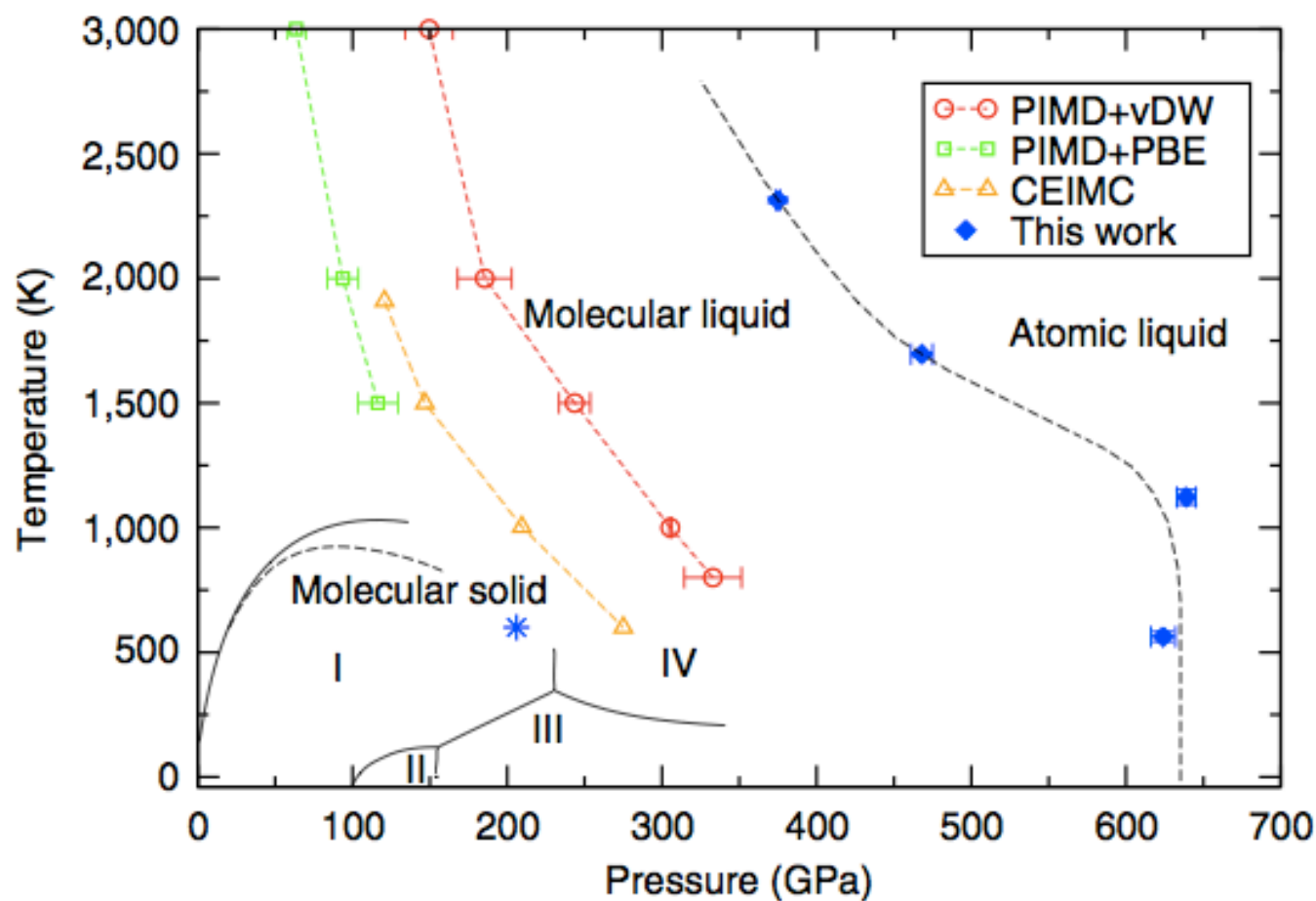
- **Goal:** to show that it is possible to automate DFT and VMC+dynamics simulations by using modeFRONTIER.
- Small system of 16 hydrogen atoms (only 8 CPUs).

- Starting from an initially optimised JDFT single determinant wave function, we want to make a dynamic like this:
- After each ionic move:
 - DFT to fill orbitals in SD with the new positions
 - Few iterations of VMC to optimise Jastrow factor.
- 1000 thousand iterations (to reach thermalisation).

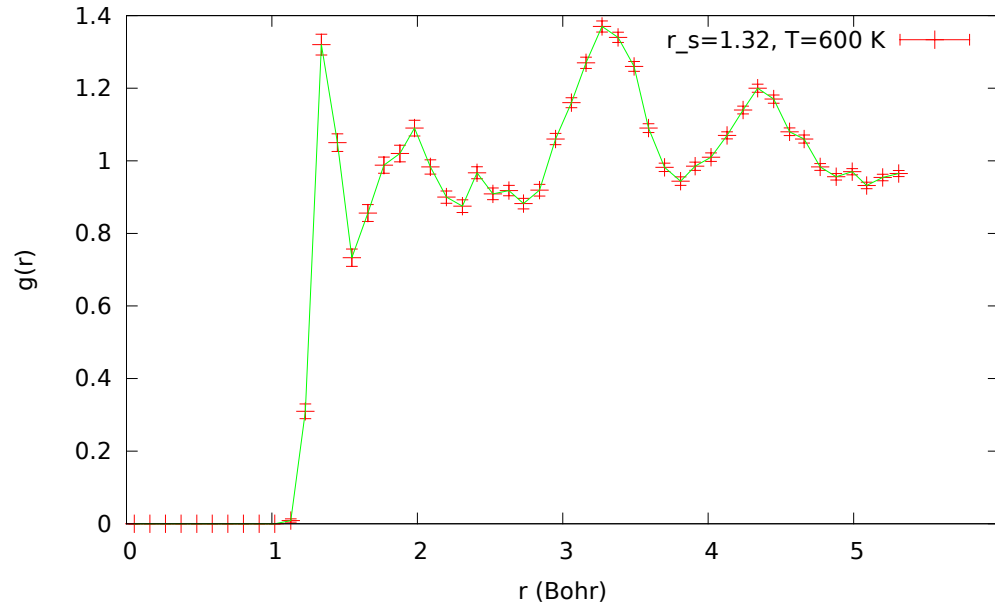
- Use of **TurboRVB** code (developed by S. Sorella et al.): DFT, VMC and dynamics packages
- J-DFT single determinant wave function
- Second-order Langevin Dynamics to sample ionic configurations within Born-Oppenheimer approximation (see G. Mazzola, S. Yunoki and S. Sorella, Nature Communications, 2014).

- First: simulations at $T=600\text{K}$ and $r_s=1.32$.
- Checked DFT and QMC energies and variance of QMC energy.
- Dynamics.
- Radial distribution function.
- Second: simulations at $T=2400\text{K}$, to check whether a liquid-liquid transition could be detected.

Sandro's phase diagram

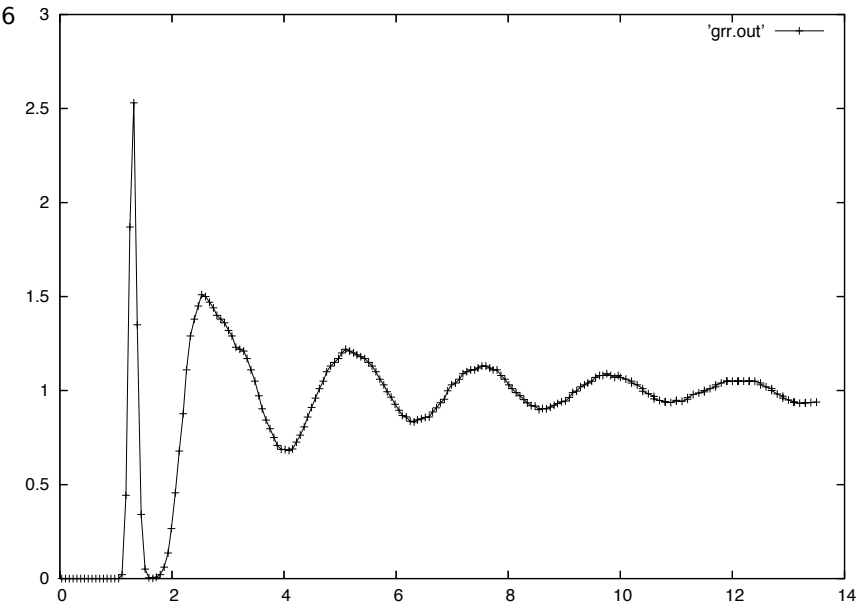


- modeFRONTIER DEMO
- Energy checks...
- Dynamics movie

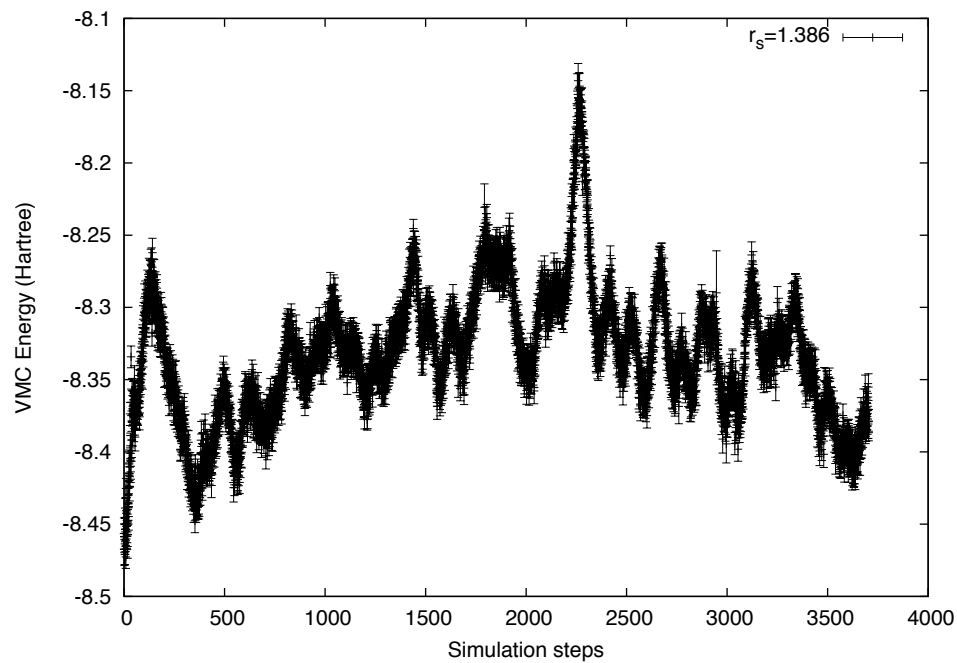


Pressure $\approx 359 \text{ GPa}$

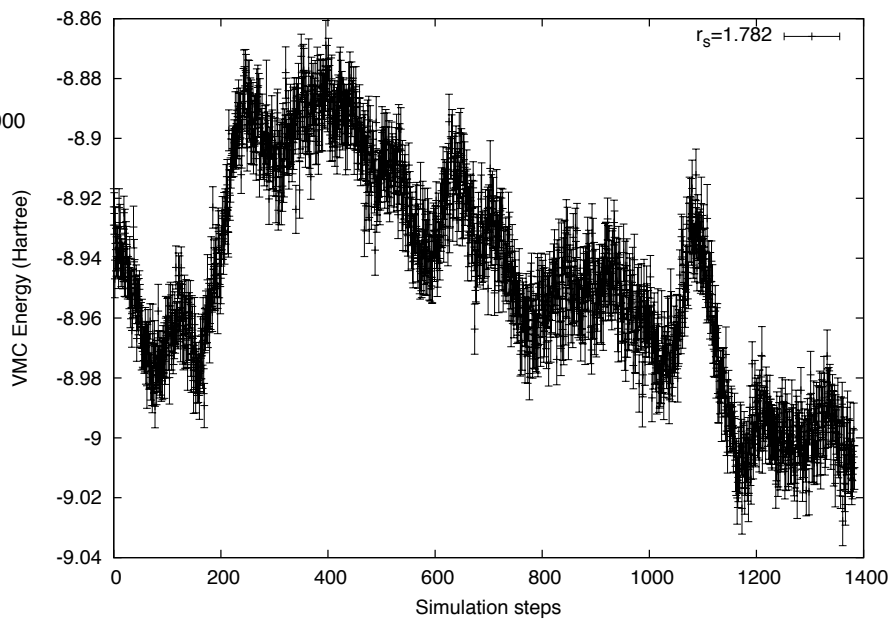
Courtesy of G. Mazzola
(Same r_s and T . $N=256 \text{ H}$)



- The idea was to look for the liquid-liquid transition, starting from two points on the molecular liquid and atomic liquid side, and see if we could detect changes in some properties like molecular peaks in the $g(r)$ or abrupt jumps in the P - r_s diagram.
- But... Unstable simulations to begin with, so more preliminary checks are necessary in this case before automating the procedure.



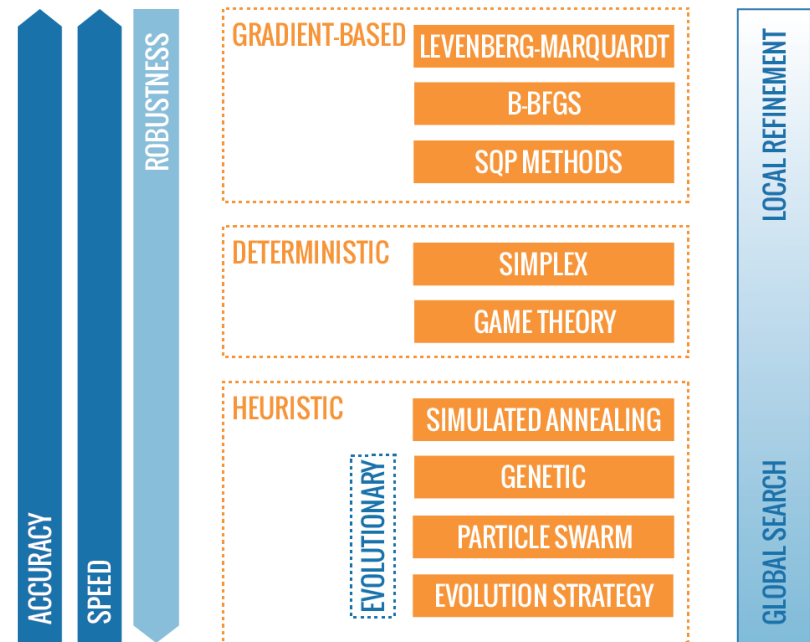
WORK IN PROGRESS



Present conclusions

- It is possible to *use modeFRONTIER to automate scientific simulation processes*
- So far, a complicated way to make a script. Effort compensated by monitor tools, reusable setups, etc.
- The **most interesting** parts are probably:
 - See the **right panel!**
 - **Possibility of** integrating different software packages

Perspectives: automation & optimisation





mode **FRONTIER**

Thank you
for your attention!

