

Centre for Data and Computational Sciences

some thoughts from an application-oriented node

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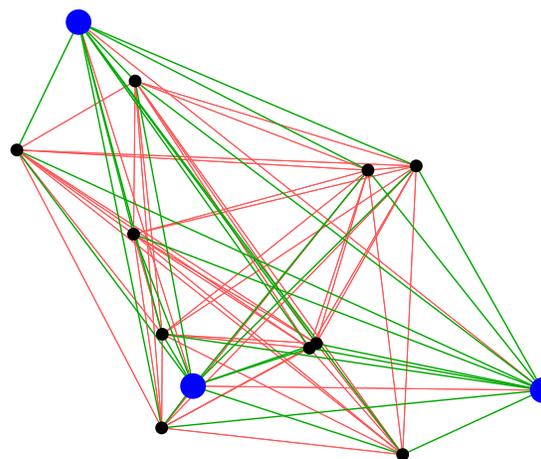
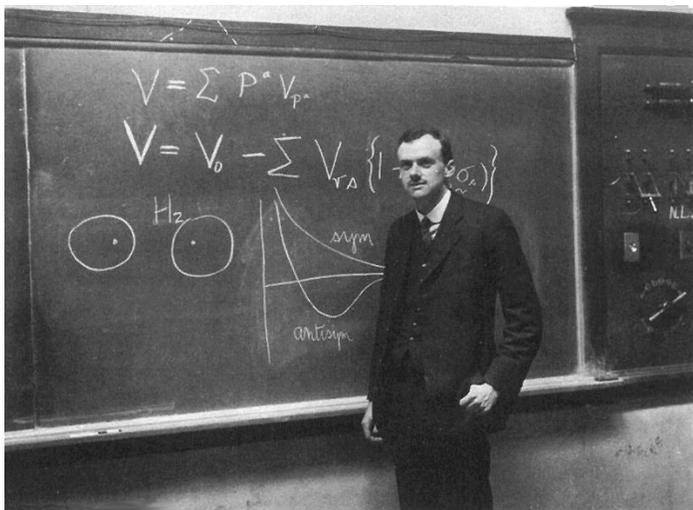
Kick-off Seminar

Thon Hotel Opera, 26th September 2019

The molecular many-body problem

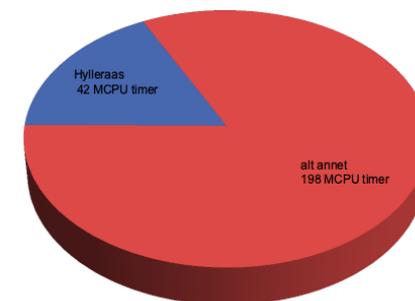
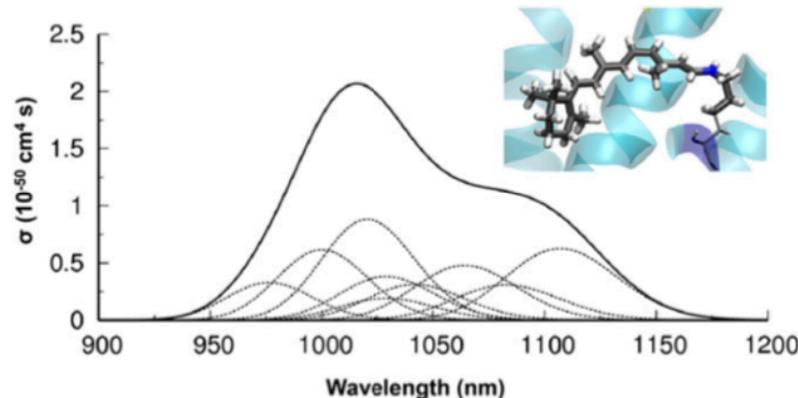
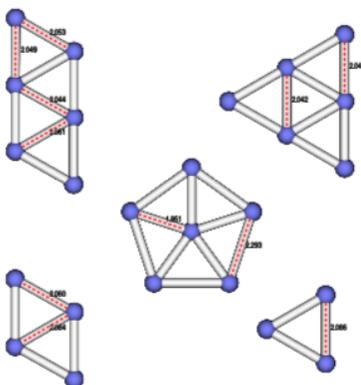
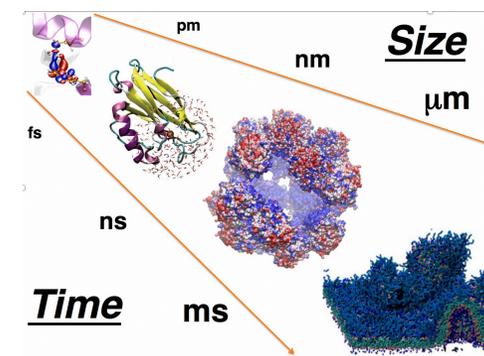
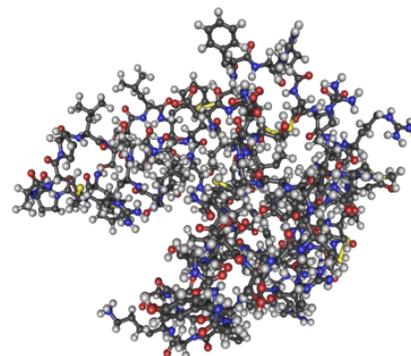
- Paul Dirac (1929):

The underlying **physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known** and the difficulty is only that the exact application of these laws leads to equations **much too complicated to be soluble**. It therefore becomes desirable that **approximate practical methods of applying quantum mechanics should be developed...**



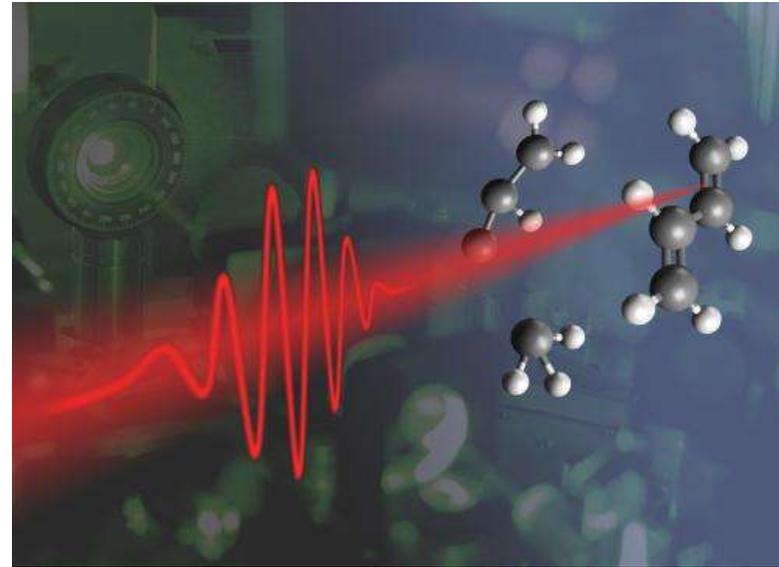
Theoretical chemistry

- **Quantum chemistry**
 - quantum mechanics applied to molecules
- **Multiscale methods**
 - complex systems up to mesoscale
- **Generic tools with wide range of applicability**
 - bonding in ultra-strong magnet fields to human infrared vision



Motivation for Hylleraas Centre

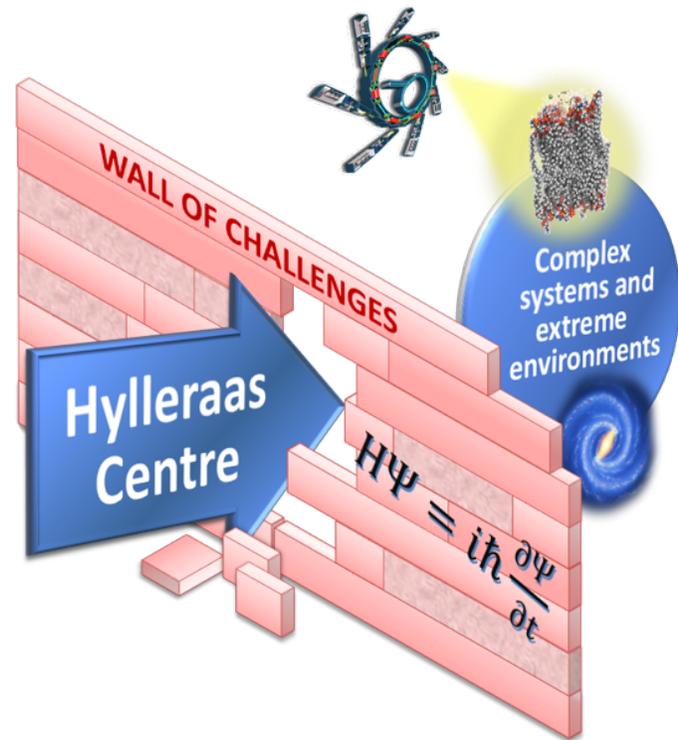
- New experimental facilities revolutionize how we study matter
 - unprecedented resolution in time and space



- Revolution in computation needed to seize new opportunities
 - we will develop, apply, and distribute the necessary computational tools

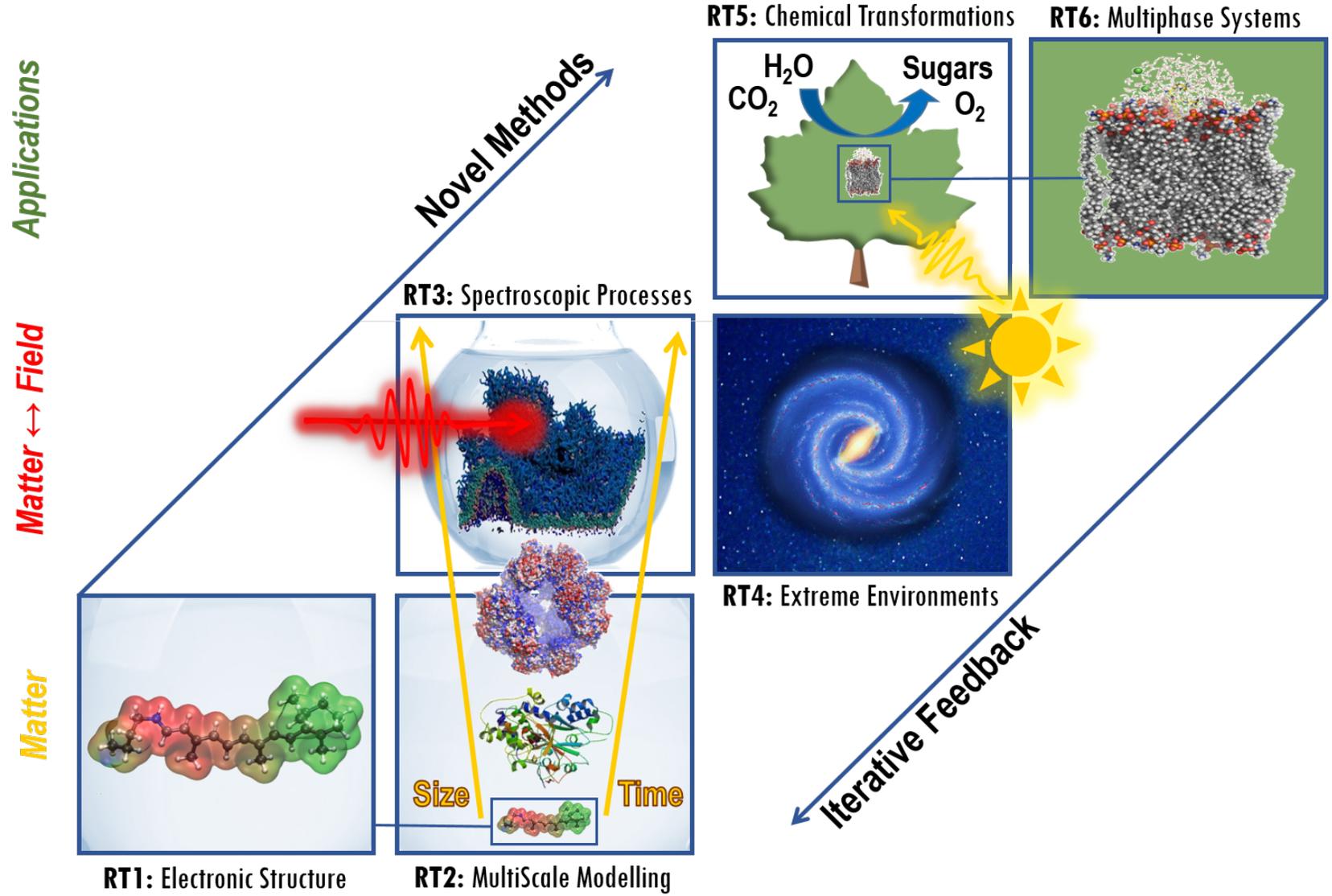
Challenges

- Millions of atoms in short laser pulses and strong fields
 - local and global processes occurring over short and long time scales
- Modeling of such processes poses a wall of challenges
 - forcing us to take fresh look at computation



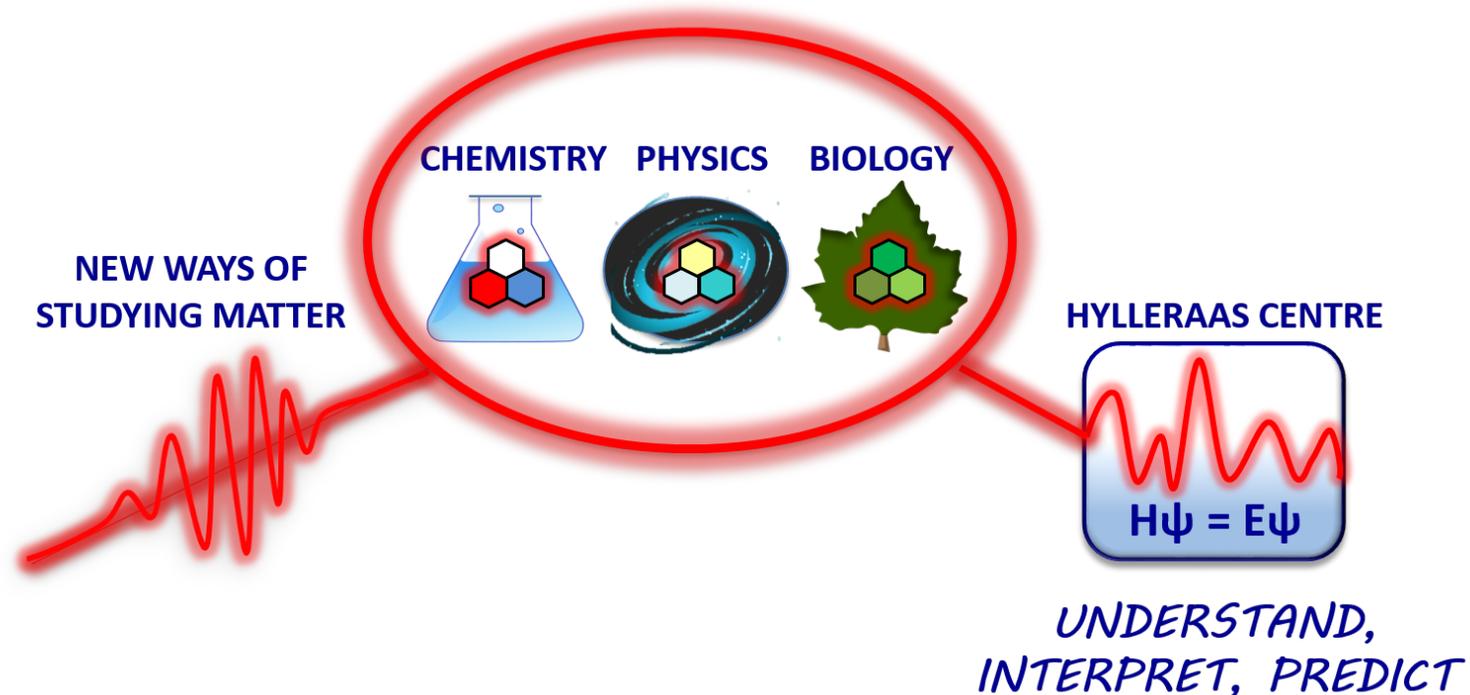
TEAR
DOWN
THE
WALL!

Research Themes



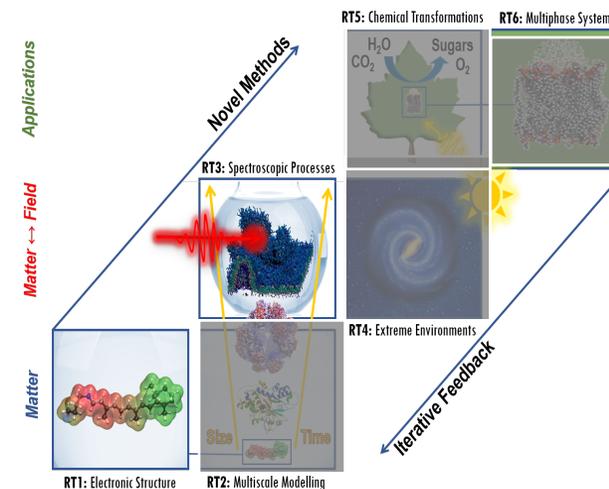
Our vision

The Hylleraas Centre will develop and apply computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments



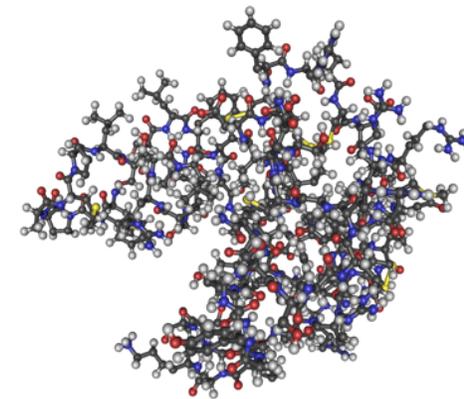
From CTCC to Hylleraas Centre

- Both centres shared between **UiO and UiT**
 - increased national impact
- CTCC had **narrower theoretical profile**
 - participation of experimental groups
- Theory groups **strengthened** in second CTCC period
 - strategic decision towards chemistry and biology
- Broad **complementary expertise**
 - Norwegian theoretical chemistry strengthen where previously weak



Production chain of theoretical chemistry

- We use **computational science to solve a physical problem of chemical relevance**
 - we propose and develop new methods and models in molecular electronic-structure theory
 - we implement these methods in advanced computer programs
 - we use these to solve problems in chemistry, physics and biology
- We are **interdisciplinary** and even **multidisciplinary**
 - we are eventually moving into the Life Science Building...



Computational science at the Hylleraas Centre

- Our work depends heavily on **computational science**
 - even data science recently (David Balcells & Riccardo De Bin)
- Interactions go back to the days of **CMA**
 - important recruitment of Simen Kvaal
- Two **ERC projects**
 - functional analysis, convex and nonlinear analysis, spectral theory
- Organized **MFO workshop 2018**
 - “Mathematical Methods in Quantum Chemistry”



Mathematisches
Forschungsinstitut
Oberwolfach



Generalized Kohn-Sham iteration on Banach spaces

J. Chem. Phys. **149**, 164103 (2018); <https://doi.org/10.1063/1.5037790>

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Department of Chemistry

The Hylleraas center of excellence in computational and theoretical chemistry is a typical example of where a large variety of algorithms for solving quantal many-body problems play a central role. These algorithms span the whole spectrum of central methods in computational science, from large eigenvalue problems to stochastic simulations, large systems of non-linear equations and systems of ordinary and partial differential equations. High-performance computing with CPU and GPUs play a central role and the applications span from material science to a fundamental understanding of reactions. Many of the research groups are involved with multi-scale problems, where an understanding of methods that apply to a certain length and energy scale and how to link different scales plays a central role. Machine learning is being used in the analysis of theoretical and experimental data.

Centre for Data and Computational Sciences

We propose to establish a center in Data Science and Computational Science at the Faculty of Mathematics and Natural Sciences. The aim is that the center becomes a leading environment in Europe both within research and education in these areas.

- Great — exactly what we want!
 - strong raison d'être
- But ...what's in it for us?
 - positions, students... ?
- What is our role?
 - how can we contribute?



(Proposed) Center for Computing and Data Sciences,
Boston University

Some experiences with setting up a centre

- The **centre vision** must be shared by all principal investigators
 - most critical point when setting up a centre
 - be prepared to drop people that do not fit
 - «The selection of such topics will depend on which researchers that choose to be part of the center»
- The **team dynamics** changes as soon as the centre becomes a reality
 - a joint battle for the centre becomes a competition for limited resources
- How do we **keep principal investigators enthusiastic** — year after year?
 - limited centre resources — can only keep so many happy
 - create and maintain ownership



Hub–node structure

- **Hub structure**
 - relations to “other centres and research groups” a challenge
 - will we only meet at the Christmas Parties and in the Annual Reports?
- **New positions**
 - 10 new positions with a strong methodological orientation with connection/responsibility towards a specific discipline/domain
 - 15–20 PhD/postdoc positions
- **What can the Hylleraas Centre can expect?**
 - one shared position at our centre one shared PhD/postdoc
 - access to expertise and students — a meeting place



- Relations to other centers and research groups
 - Internal centers: Oslo center for Biostatistics and Epidemiology (OCBE), the Joint Centre for Bioinformatics in Oslo, the Hylleraas center of excellence in computational and theoretical chemistry and the Rosseland Centre for Solar Physics.
 - Other research groups and centers at the university outside MN.
 - Centers outside UiO: NR, Simula, Sintef, Nora-centers, Startup-Lab.

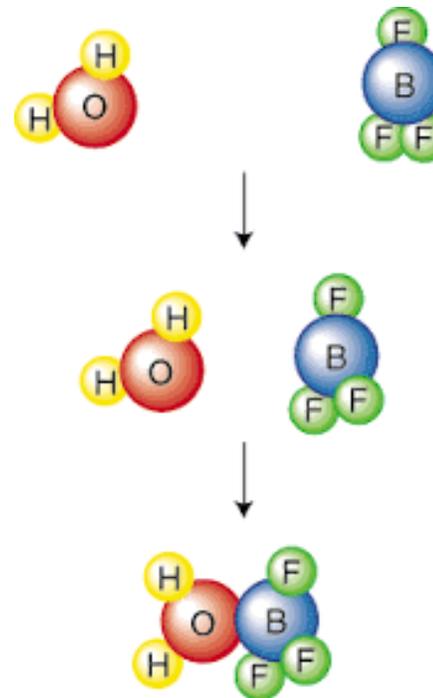
Grumblings from the nodal hinterland

- We are already **busy**
 - must be sure that we get as much back from participation as we put in...
- We are **jacks of all trades**
 - but perhaps more knowledgeable than you suspect
 - we have access to literature, internet resources, and our colleagues
 - But we could certainly gain from a personal relationship to experts
- Helping us in a meaningful way will be **time consuming**
 - fruitful collaboration takes time — are we sufficiently committed?
- Mathematics and informatics are **enormous fields of research**
 - will your particular expertise and interests match our needs and interests?



Mechanisms at the Hylleraas Centre

- **Use resources as a centre glue**
 - do not spend all resources on positions
 - maintain generous program visits, workshops, conferences
- **Schedule shared regular events**
 - seminars, annual meetings, social events
- **Make each year different**
 - schedule years of planned activities within some chosen focus area
- **Involve young researchers**
 - young parliament, participation in leadership, responsibility for regular events, career development
- **Efficient means of communication**
 - videoconference rooms for joint presentations and teaching at different locations



Concluding remarks and questions

- Yes, we are **interested** and **even enthusiastic** about this!
 - but how can we ensure that this is not just for Mathematics and Informatics?
 - what is our role — what do we gain and what do we give?
- But, we have our **preexisting commitments** to the research council and home institutions
 - how will teaching be shared?
 - what recruitments will be allocated to us?
- Our influx of **students** with the right profile is small
 - how can we share students and young researchers?
 - will students in Data Science and Computational Science take master with us?

