Welcome to **RDMFT2022**

International workshop on Reduced Density Matrix Functional Theory: Improving its Foundations and Extending its Scope

Carlos L. Benavides-Riveros, Hardy Gross & Christian Schilling

cecam
Centre Européen de Calcul Atomique et Moléculaire

ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS

The one-body reduced density matrix

$$\gamma(\vec{x},\vec{y}) = \int \Psi(\vec{x},\vec{x}_2,...,\vec{x}_N)\Psi^*(\vec{y},\vec{x}_2,...,\vec{x}_N)d\vec{x}_2\cdots d\vec{x}_N$$

contains the density $\rho(\vec{x}) = \gamma(\vec{x},\vec{x})$

but also coherence and entanglement

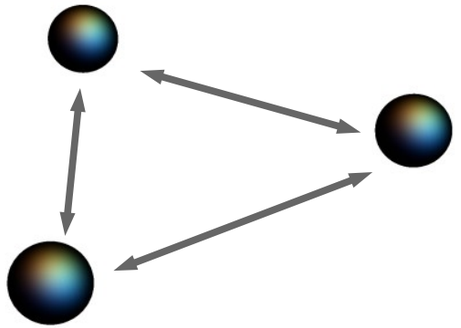
$$\gamma(\vec{x},\vec{y}) = \sum_i n_i\phi_i(\vec{x})\phi_i^*(\vec{y})$$

$$\hat{H} = \hat{h} + \hat{W}$$

$$\hat{h} = \sum_i \hat{h}_i \qquad \hat{W} = \sum_{i<j} \hat{W}_{ij}$$

1-particle operators

2-particle operator



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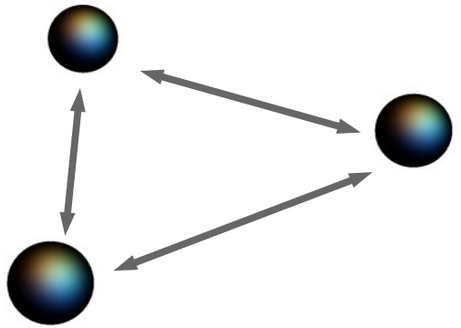

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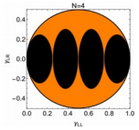
1-particle operators

2-particle operator

$$E(\hat{h}) = \min_{\gamma \in} [\langle \hat{h}, \gamma \rangle + \mathcal{F}(\gamma)]$$



$$\mathcal{F}(\gamma) = \min_{|\Psi\rangle \to \gamma} \langle \Psi | \hat{W} | \Psi \rangle$$

RDMFT

fermions (1975)

T > 0 (2015)

bosons, ultracold gases (2020)

machine learning (2021)

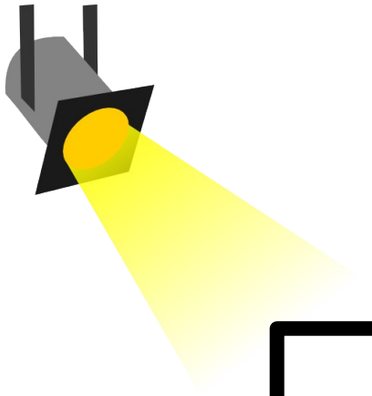
time-dependent RDMFT (2008)

superconductors (2019)

excited states (2021)

relativistic fermionic systems (2022)

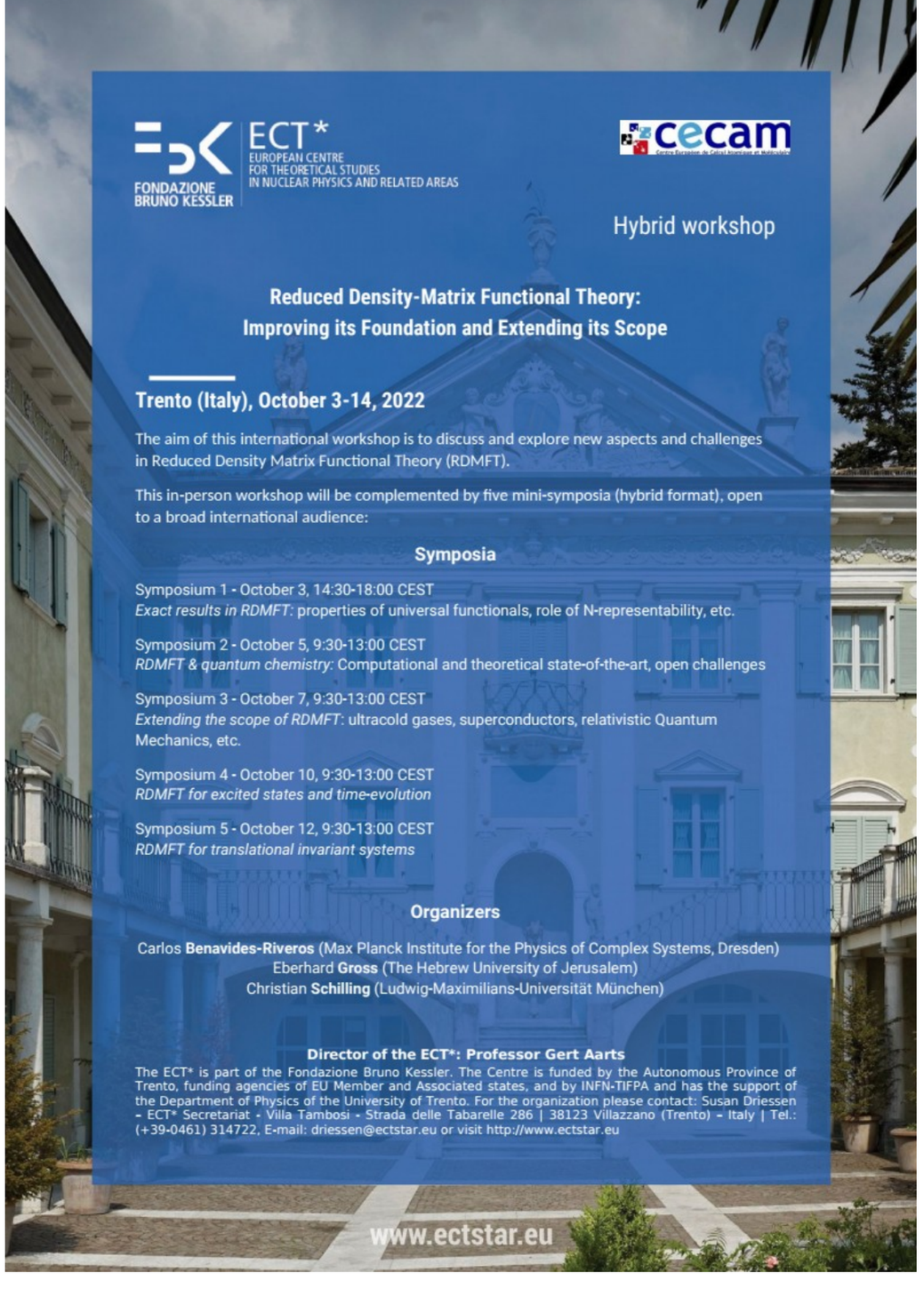
(original) motivation of RDMFT2022



improve the foundations of RDMFT

extend the scope of RDMFT

in an intensive & informal meeting



FONDAZIONE BRUNO KESSLER

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Hybrid workshop

Reduced Density-Matrix Functional Theory: Improving its Foundation and Extending its Scope

Trento (Italy), October 3-14, 2022

The aim of this international workshop is to discuss and explore new aspects and challenges in Reduced Density Matrix Functional Theory (RDMFT).

This in-person workshop will be complemented by five mini-symposia (hybrid format), open to a broad international audience:

Symposia

Symposium 1 - October 3, 14:30-18:00 CEST
Exact results in RDMFT: properties of universal functionals, role of N-representability, etc.

Symposium 2 - October 5, 9:30-13:00 CEST
RDMFT & quantum chemistry: Computational and theoretical state-of-the-art, open challenges

Symposium 3 - October 7, 9:30-13:00 CEST
Extending the scope of RDMFT: ultracold gases, superconductors, relativistic Quantum Mechanics, etc.

Symposium 4 - October 10, 9:30-13:00 CEST
RDMFT for excited states and time-evolution

Symposium 5 - October 12, 9:30-13:00 CEST
RDMFT for translational invariant systems

Organizers

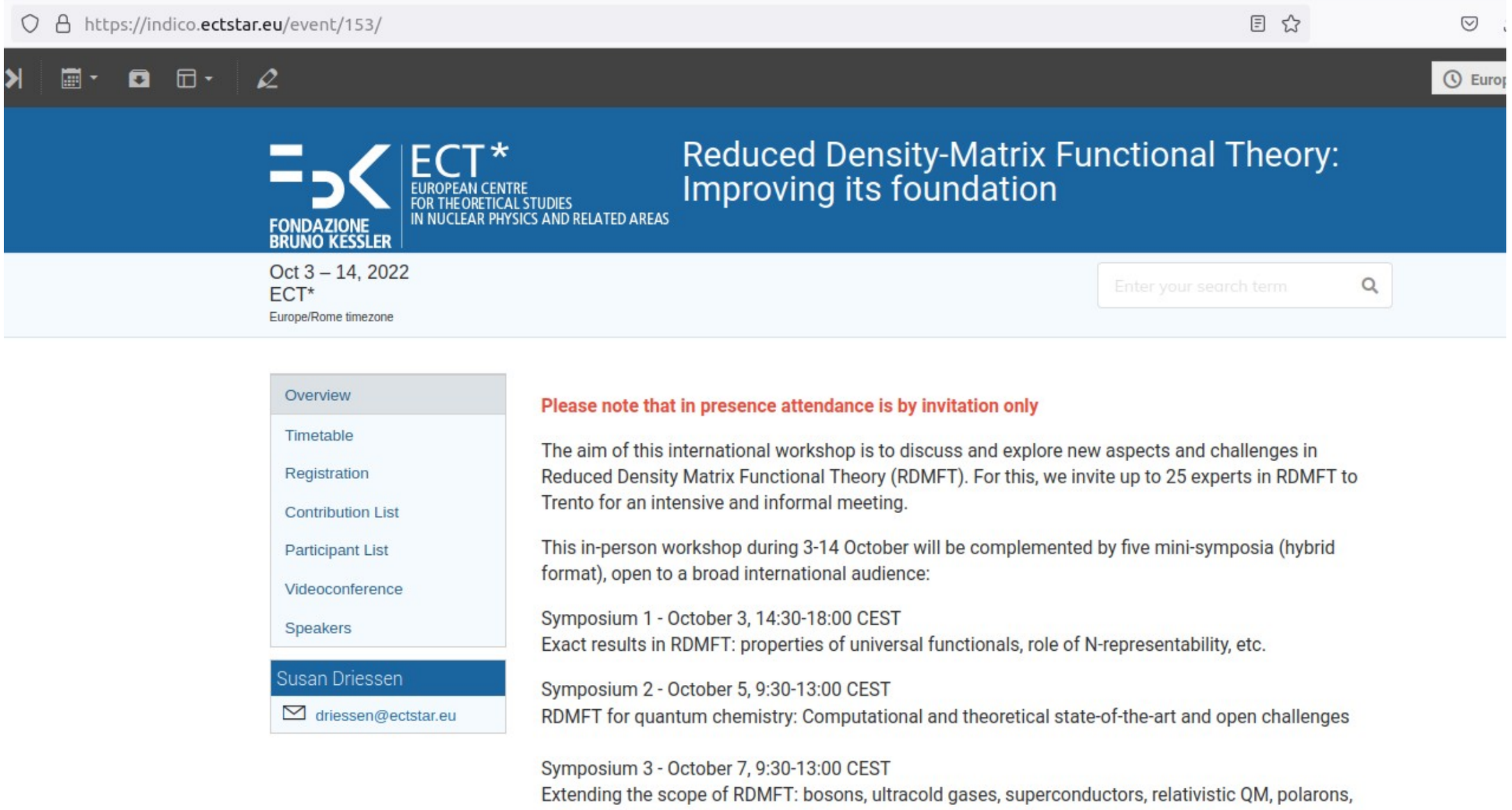
Carlos **Benavides-Riveros** (Max Planck Institute for the Physics of Complex Systems, Dresden)
Eberhard **Gross** (The Hebrew University of Jerusalem)
Christian **Schilling** (Ludwig-Maximilians-Universität München)

Director of the ECT*: Professor Gert Aarts

The ECT* is part of the Fondazione Bruno Kessler. The Centre is funded by the Autonomous Province of Trento, funding agencies of EU Member and Associated states, and by INFN-TIFPA and has the support of the Department of Physics of the University of Trento. For the organization please contact: Susan Driessen - ECT* Secretariat - Villa Tambosi - Strada delle Tabarelle 286 | 38123 Villazzano (Trento) - Italy | Tel.: (+39-0461) 314722, E-mail: driessen@ectstar.eu or visit http://www.ectstar.eu

www.ectstar.eu

indico.ecstar.eu/event/153



Susan Driessen
driessen@ectstar.eu

Timetable

10:00

Registration
Hall Rustico 10:00 - 10:30

Introduction
*Sala Leonardi, ECT** 10:30 - 11:00

11:00

Coffee break
11:00 - 11:30

Welcome *Christian Schilling & Carlos Benavides-Riveros*

12:00

*Sala Leonardi, ECT** 11:30 - 13:00

13:00

Lunch
13:00 - 14:29

14:00

Symposium 1: Exact results in RDMFT *Carlos Benavides-Riveros*

DFT, RDMFT, and the challenge of strong correlations *Eberhard Gross*
*Sala Leonardi, ECT** 14:30 - 15:00

15:00

Density Functional Theory Transformed into a One-electron Reduced Density Matrix Functional Theory for the Capture Static Correlation
David Mazziotti

One-body Reduced Density-matrix Functional Theory for the Canonical Ensemble *Sarina Sutter*
*Sala Leonardi, ECT** 15:30 - 16:00

16:00

Coffee break
16:00 - 16:30

Convex N-Representability *Federico Castillo*
*Sala Leonardi, ECT** 16:30 - 17:00

17:00

Relating the pure and ensemble density matrix functional *Christian Schilling*
*Sala Leonardi, ECT** 17:00 - 17:30

Implications of pinned occupation numbers for natural orbital expansions *Tomasz Maciazek*
*Sala Leonardi, ECT** 17:30 - 18:00

18:00

5 Symposia

Symposium 1: exact results in RDMFT (Mon)

Symposium 2: RDMFT for quantum chemistry (Wed)

Symposium 3: bosons, ultracold gases, superconductors (Fri)

Symposium 4: conceptual aspects of RDMFT (Mon)

Symposium 5: excited states, time evolution, and more (Wed)

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20min + 10min Q&A (mixed audience!)

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20min + 10min Q&A (mixed audience!) **open challenges and ideas**

During the next 2 weeks

11:00 – 11:30: coffee break

13:00 – 14:30: lunch

16:00 – 16:30: coffee break

Wednesdays nights: dinner (Ristorante Ca dei Gobj and tba)

questions & technical difficulties ?

➟ talk to Susan,

Carlos, Hardy & Christian

Enjoy

RDMFT2022!