Toward predictive modeling of Inertial Confinement Fusion plasmas

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In collaboration with Christopher Makait, Hanno Kählert, Erik Schroedter, Daniels Krimans, Jan-Philip Joost (Kiel)

With contributions from S. Hu, V. Karasiev (U Rochester),
T. Dornheim, Zh. Moldabekov, J. Vorberger, P. Hamann (HZDR),

„DPG-Frühjahrstagung“, Erlangen, März 2026

pdf of talk at https://www.itap.uni-kiel.de//theo-physik/bonitz/talks.html

Recent breakthroughs in ICF a the NIF

H. Abu-Shawareb *et al*, "Lawson criterion for ignition exceeded in an inertial fusion experiment," Phys. Rev. Lett. **129**, 075001 (2022). [August 8]

H. Abu-Shawareb *et al*, "Achievement of Target Gain Larger than Unity in an Inertial Fusion Experiment", Phys. Rev. Lett. **132**, 065102 (2024) [subm. 27 Oct 2023, published Feb. 5 2024]

413 and 291 citations (March 10 2025)

2022 Dawson Award for Excellence in Plasma Physics Research for „NIF's Burning Plasma Team"

DOE Press conference on Dec 13 2022 (quoting „historic shot" of Dec 5): global news response

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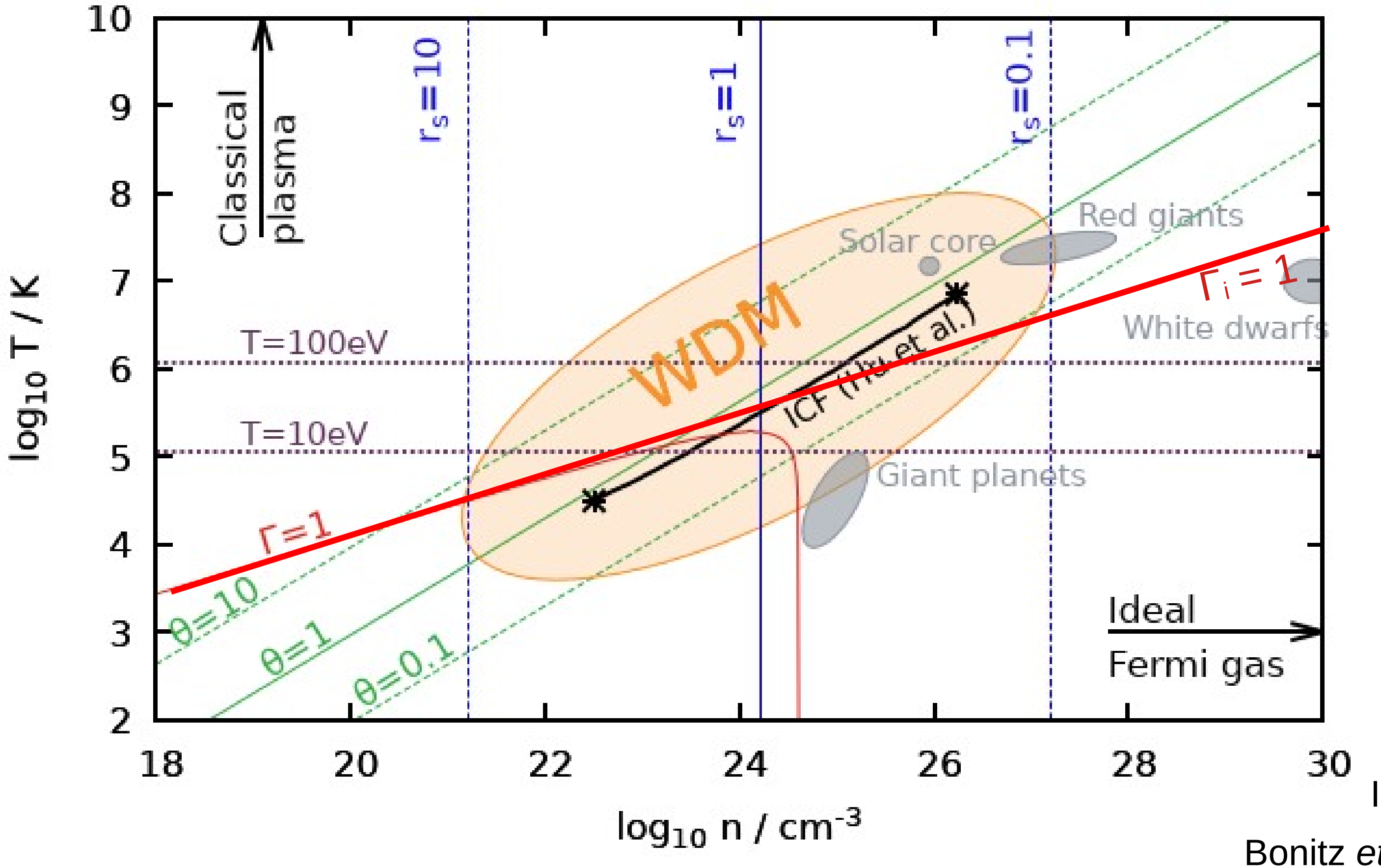
Astonishing impact on politics and research world-wide: many startups + public investment

US: DOE Fusion Science & Technology Roadmap, > $ 9 B private investments, public infrastructure by mid 2030s (magnetic fusion and ICF)

Germany: novel „High-tech agenda“ lists fusion as one of 6 focus areas
Action plan of federal government „Germany on track towards a fusion power plant“
Goal: „build the first fusion power plant in Germany“ (demo)
Public Investment: € 1.7B until 2029
Magnetic fusion (stellarator) and ICF

Plasma parameters at ICF conditions



$$\Theta = \frac{k_B T}{E_F}$$ quantum degeneracy

$$\Gamma_i = \frac{d}{k_B T}$$ ion coupling

$$r_s = \frac{d}{a_B}$$ el. coupling (T=0)

$$\Gamma = \frac{e^2}{d k_B T \frac{2\sigma+1}{n\Lambda^3} I_{3/2}(\beta\mu)}$$

generalized el. coupling par.

ICF path: Hu *et al.* Phys. Plasmas 2015

Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Warm dense matter and ICF: challenges

Challenges:

- mix of condensed matter and plasma phases
- condensed matter at high temperature (not ground state)
- plasma partially ionized
- strong many-particle effects, quantum screening, bound state renormalization
- quantum and spin effects of electrons (delocalization, exchange, Pauli blocking)
- non-uniformities: shock waves, hydrodynamic instabilities
- non-Maxwellian ions
- laser-matter interaction, coupling to radiation, nuclear reactions

How accurate are Radiation-hydro simulations for ICF?

„Hydra“ code

Known: - Approximate input of equation of state (SESAME), transport (DFT data),
- nuclear rates
- in standard hydrodynamics: no ionic correlations, no el. Quantum effects
- no non-Maxwellian effects

Unknown: magnitude of statistical errors
magnitude of systematic errors
validity limits
deviations from experiment

predictive capability?

Warm dense matter and ICF: novel opportunities

Dramatic recent progress in **WDM/ICF experiments**, in particular, at the NIF

Progress in **WDM diagnostics**, accuracy, e.g., X-ray Thomson scattering (XRTS) for many materials

Model-free high precision analysis of XRTS data (temperature diagnostic)
T. Dornheim *et al.,* Nat. Comm. Phys. **13**, 7911 (2022), Phys. Plasmas **30**, 042707 (2023)

Progress in theory and simulations: traditional (hydrodyamics, kinetic theory) and more recent methods: DFT, TDDFT, Green functions, quantum Monte Carlo

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Progress in theory and simulations: traditional (hydrodyamics, kinetic theory) and more recent methods: DFT, TDDFT, Green functions, quantum Monte Carlo

Novel opportunity: use accurate, predictive simulations as benchmark and perform Fermionic PIMC downfolding

Recent breakthroughs in first-principles/predictive QMC simulations for WDM in our group

Physics Reports **744**, 1-86 (2018)

The uniform electron gas at warm dense matter conditions

Tobias Dornheim [1], Simon Groth [1], Michael Bonitz *
Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 15, 24098 Kiel, Germany

PHYSICAL REVIEW LETTERS **121,** 255001 (2018)

Ab initio Path Integral Monte Carlo Results for the Dynamic Structure Factor of Correlated Electrons: From the Electron Liquid to Warm Dense Matter

T. Dornheim,[1] S. Groth,[1] J. Vorberger,[2] and M. Bonitz[1]
[1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, D-24098 Kiel, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany

PHYSICAL REVIEW E **108**, 055212 (2023)

Equation of state of partially ionized hydrogen and deuterium plasma revisited

A. V. Filinov * and M. Bonitz †
Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstraße 15, 24098 Kiel, Germany

Quantum Monte Carlo simulations for dense H*

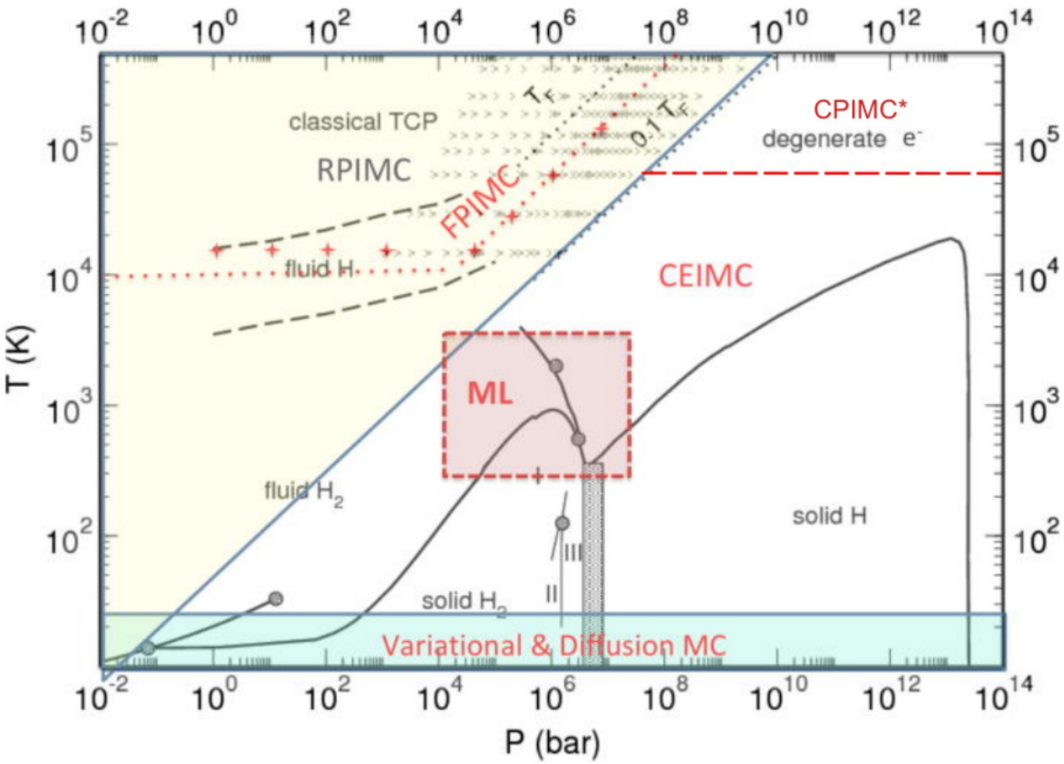


FIG. 8. Applicability range of different simulation methods across the hydrogen phase diagram. RPIMC: restricted PIMC, extends to about $0.1\,T_F$, Sec. III E 4, CEIMC: coupled electron-ion Monte Carlo, Sec. III F, FPIMC: fermionic PIMC, extends to about $0.5\,T_F$ and was applied to temperatures above 10 000 K, Sec. III E 5. ML denotes region fit by QMC-based machine learning force fields in Ref. 206 and also the region where CEIMC has been applied. Red pluses show FPIMC simulation points from Ref. 115 that mark the border of what is feasible today. Light black crosses show regions covered by the RPIMC database[114]. The other lines are introduced in Fig. 4.

CPIMC: high degeneracy, complementary to FPIMC

*M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024)

Updated version from Vorberger *et al.*, „Roadmap for Warm Dense Matter Physics“, 2026

Benchmarking RPIMC, MD for dense H: Equation of state*

Average sign of fermionic PIMC

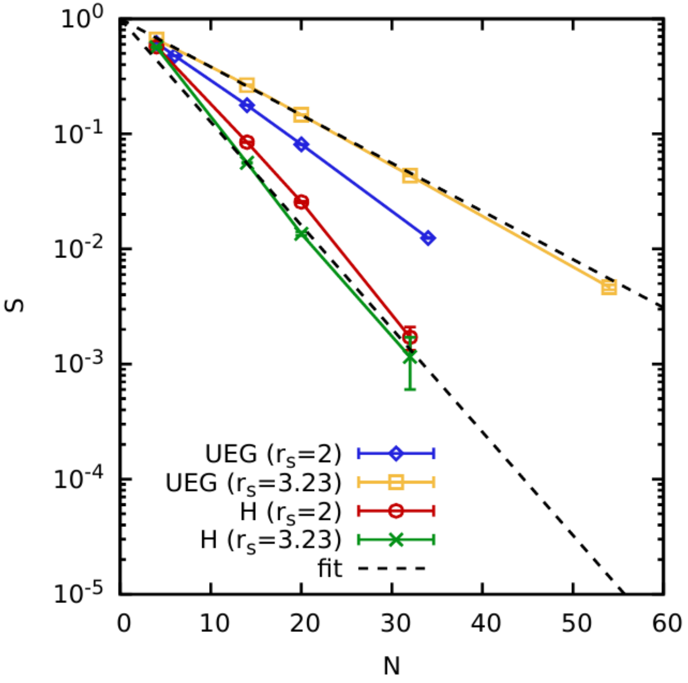
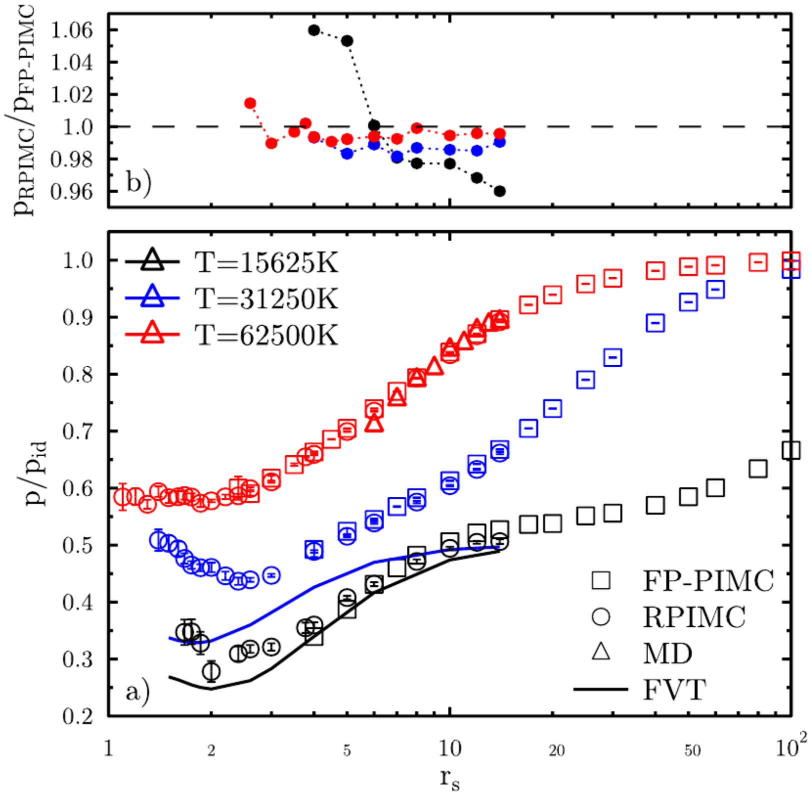


FIG. 10. Average sign S as a function of the number of electrons N at the electronic Fermi temperature $\Theta = 1$, for $r_s = 2$ ($\rho = 0.34\,\mathrm{g/cm^3}$, $T = 12.53\,\mathrm{eV}$) and $r_s = 3.23$ ($\rho = 0.08\,\mathrm{g/cm^3}$, $T = 4.80\,\mathrm{eV}$). The dashed black lines show exponential fits to the PIMC data, cf. Eq. (70). Reproduced from Ref. 149 with the permission of the authors.

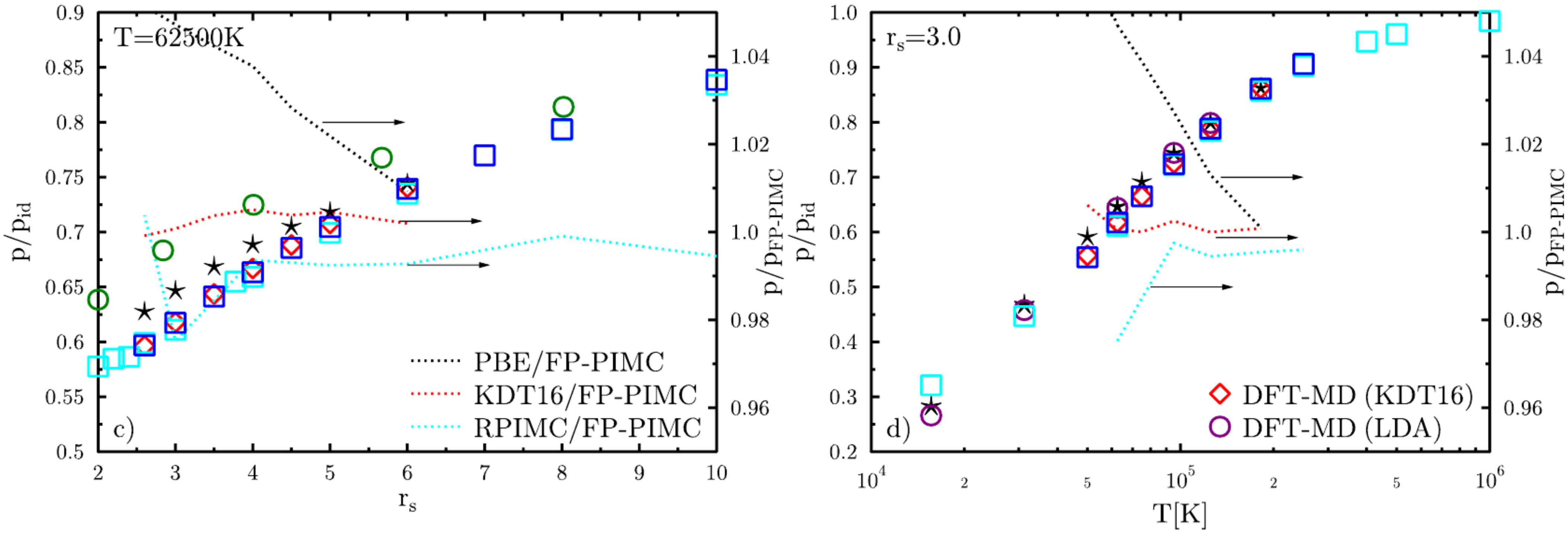


RPIMC validated by fermionic PIMC

*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)

M. Bonitz *et al.*, Phys. Plasmas 2024

Benchmarking DFT, Average atom simulations for dense H*



Dotted lines with arrows (right axes):
relative error compared to FPIMC

*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)

Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

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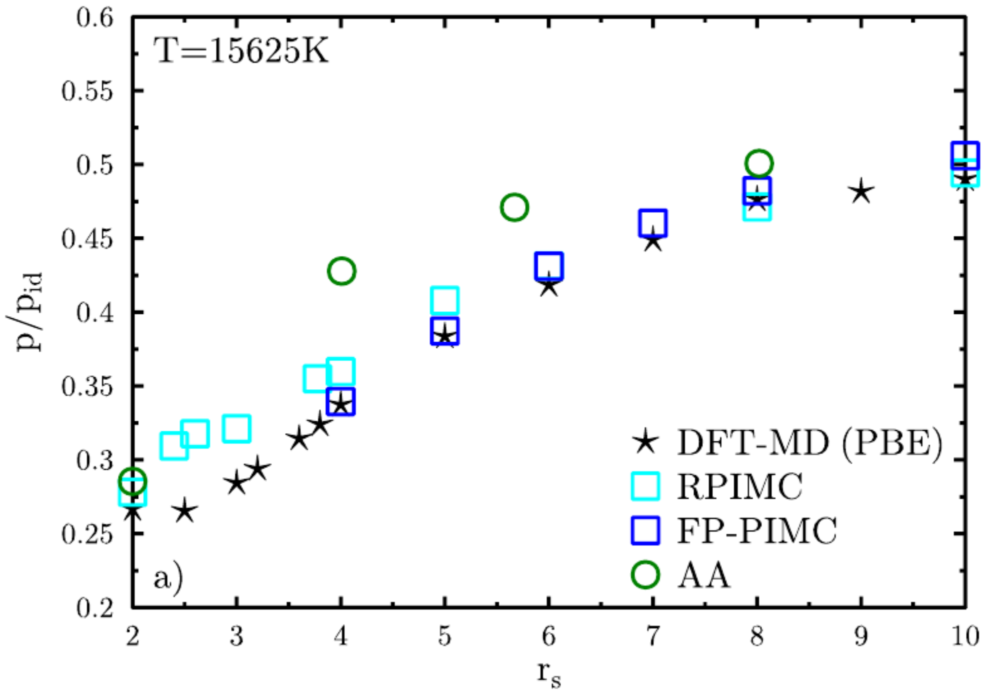

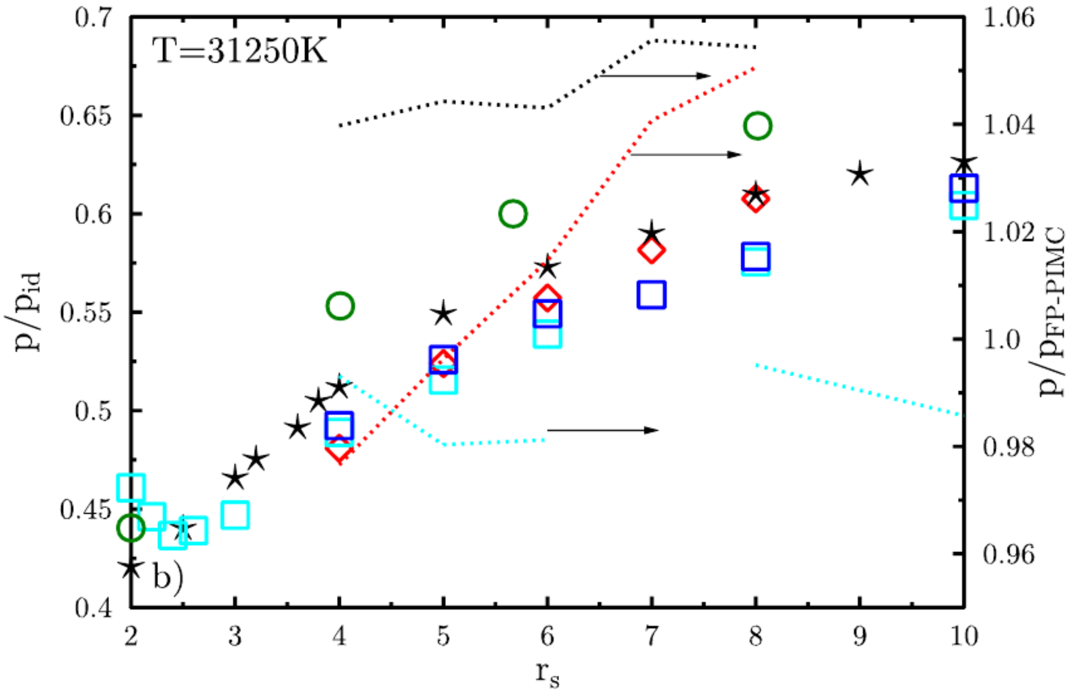

*A.Filinov and M. Bonitz, PRE **108**, 055212 (2023)
Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024)

Dotted lines with arrows (right axes): relative error compared to FPIMC

FPIMC downfolding: Kohn-Sham-DFT

Exact theory

Two exact Formulations W different resolution

Path integral representation

Density functional representation*, exact E_{xc}

Practical implementation

MC integration still exact, with statistical errors

Approximation: choice of approximate E_{xc}

„Measurement“ microscopic observable [e.g., **g(r), S(k)**] for identical parameters

Simulation result (**function**) as exact benchmark

* Hohenberg-Kohn theorems

FPIMC downfolding: Kohn-Sham-DFT

Two exact
Formulations
W different resolution

Practical
implementation

„Measurement“
microscopic observable
[e.g., **g(r), S(k)**] for
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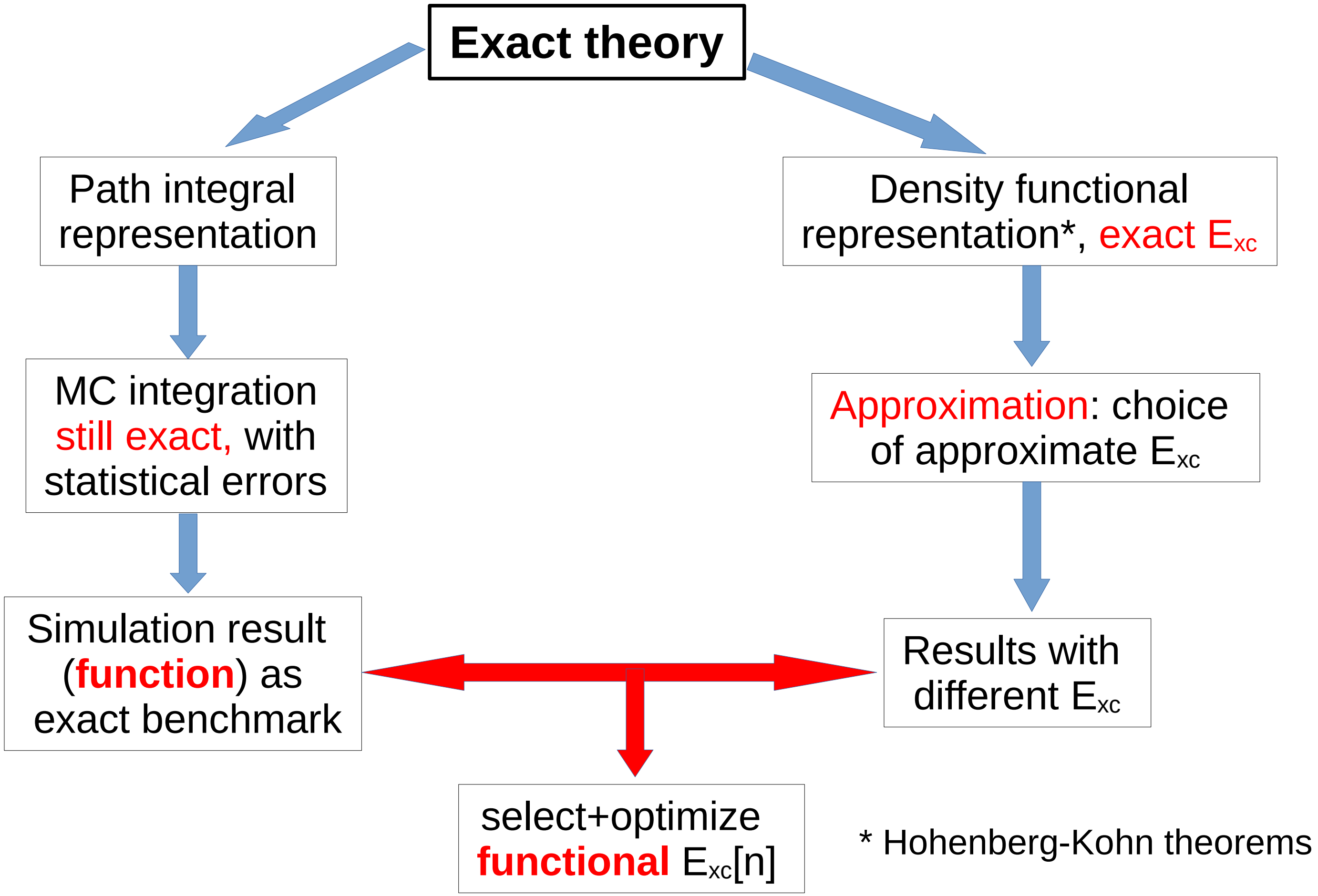


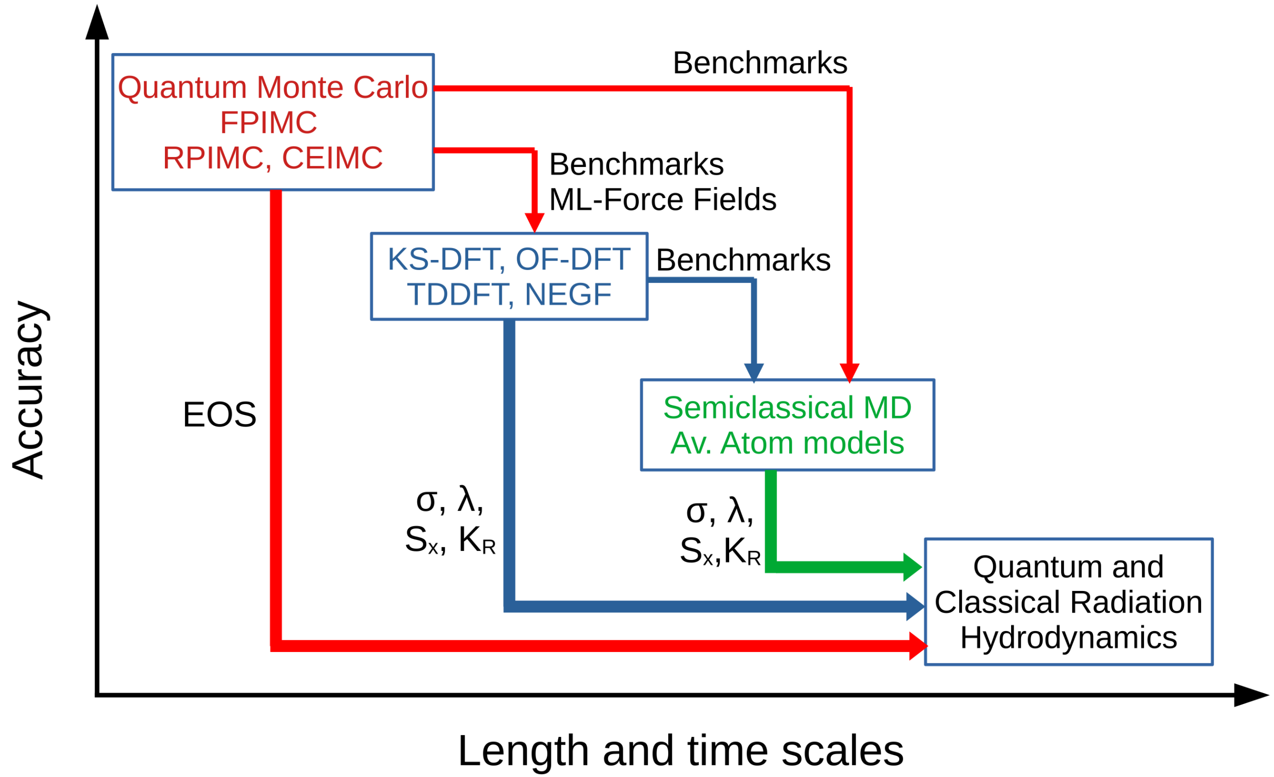
FPIMC „downfolding“ + smart combination of methods

Starting from predictive simulations (Fermionic PIMC)

→ selection of most accurate approximations of lower level models

→ reduction of resolution + increase of accessible r- and t-scales +

→ preservation of acceptable accuracy



Bonitz *et al*., Phys. Plasmas **31**, 110501 (2024); Bonitz *et al*., to be published in Phys. Plasmas (2026)

FPIMC „downfolding“ + smart combination of methods for ICF

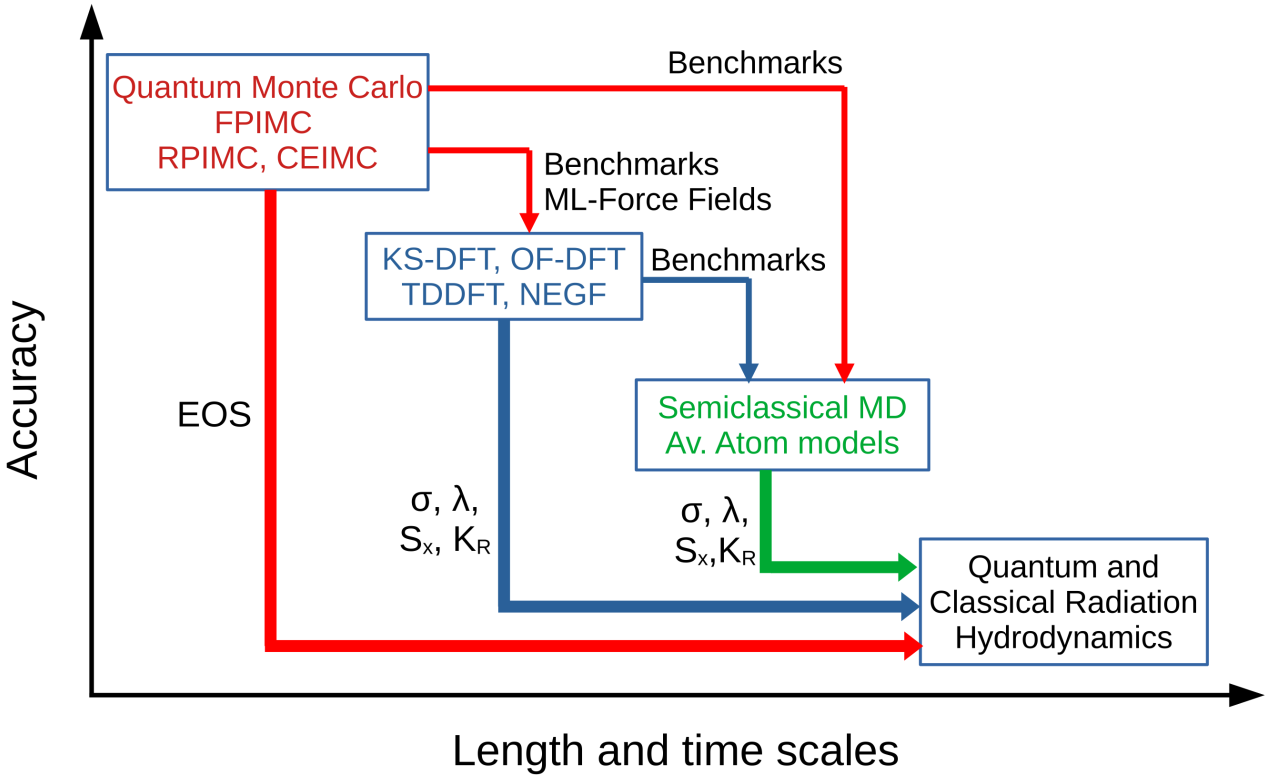
The way to go:
combination of methods

Hydro simulations indispen-Sible to cover relevant scales and complexity

with present approach:

- needed input can be improved substantially
- limitations can be better quantified

- **predictive simulations will become possible**



* M. Bonitz *et al.*, Phys. Plasmas **31**, 110501 (2024); Bonitz *et al.*, to be published in Phys. Plasmas (2026)

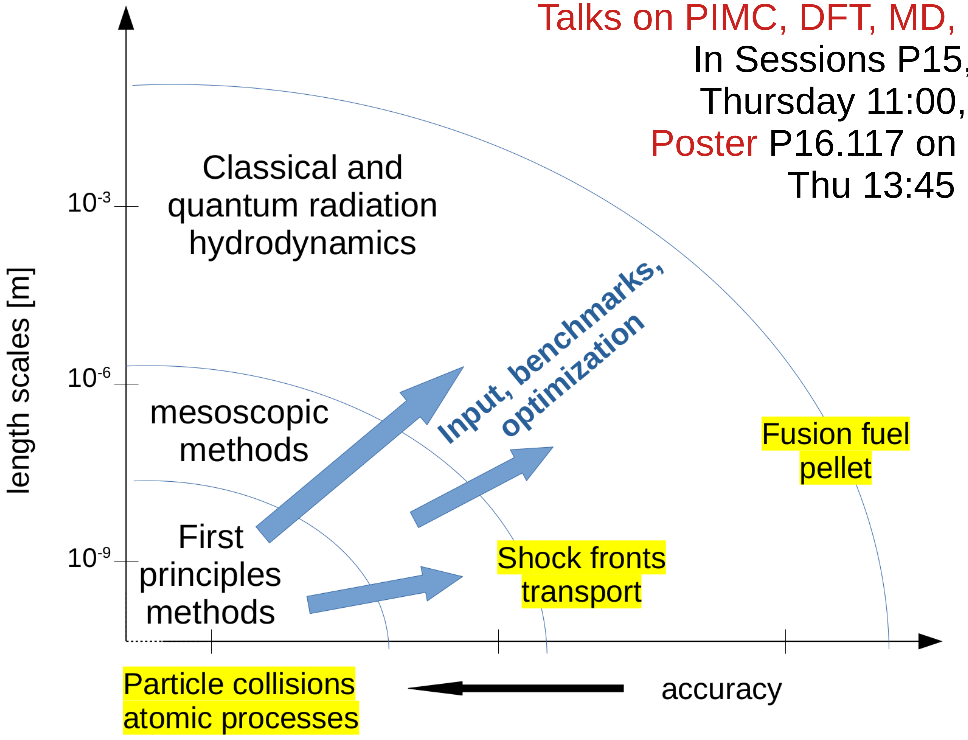
Summary

Needed:

Combine radiation hydro with more advanced simulations on different scales

Achieve predictive capability for ICF simulations

Talks on PIMC, DFT, MD, hydro
In Sessions P15, P18,
Thursday 11:00, 16:15
Poster P16.117 on NEGF
Thu 13:45



Verbundprojekt (in „Basistechnologien für die Fusion“), Koordinator: M. Bussmann

from M. Bonitz, T. Dornheim and R. Redmer, the Innovation Platform ISSUE 25 (2026)