DFT (or ?) and EFT: Recent developments and ideas

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*Low-energy nuclear theory get-together*

ORNL, December, 2017

Collaborators: S. Bogner (MSU), A. Dyhdalo (OSU), R. Navarro-Perez (OU), N. Schunck (LLNL), Y. Zhang (OSU) plus discussions with T. Papenbrock (UT) and many others
Outline

Viewpoint: nuclear reduction and emergence

(Preliminary) results from new DME implementation

How to proceed with EFT for DFT (or alternative)?

Extra: Statistical tools and recent RKE potentials
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Extra: Statistical tools and recent RKE potentials
Hierarchy of nuclear degrees of freedom

LQCD

constituent quarks

ab initio

CI

DFT

collective models

Physics of Hadrons

Physics of Nuclei

Degrees of Freedom

Energy (MeV)

scale separation

940 neutron mass

140 pion mass

8 proton separation energy in lead

1.12 vibrational state in tin

0.043 rotational state in uranium

Reductive and Emergent ⇒ EFT (see 2017 Saclay workshop)

Where does EDF/DFT fit in?
Hierarchy of nuclear degrees of freedom

- **LQCD**
  - quarks, gluons
  - 940 neutron mass
- **ab initio**
  - baryons, mesons
  - 140 pion mass
- **Cl**
  - protons, neutrons
  - 8 proton separation energy in lead
- **DFT**
  - nucleonic densities and currents
  - 1.12 vibrational state in tin
- **collective models**
  - collective coordinates
  - 0.043 rotational state in uranium

**Multiple phenomenologies**
- Constituent quarks
- Meson exchange models
- Cluster models
- Collective models
- Nuclei as Fermi liquids
- Nuclear pairing

**Resolution**

Reductive and Emergent =⇒ EFT (see 2017 Saclay workshop)

“Behind every successful emergent phenomenology there is an EFT (or EFTs) waiting to be uncovered”

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Hierarchy of nuclear degrees of freedom

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Hierarchy of nuclear degrees of freedom

- **LQCD**
- **ab initio**
- **CI**
- **DFT**
- **collective models**

**Reductive and Emergent** ⇒ **EFT** (see 2017 Saclay workshop)

- Chiral quark model
- Chiral EFT: nucleons, \([\Delta’s,]\) pions; [within HO basis]
- Pionless EFT: nucleons only (low-energy few-body) or nucleons and clusters (halo)
- EFT for deformed nuclei: systematic collective dofs (Papenbrock et al.)
- EFT at the Fermi surface (Landau-Migdal theory; superfluidity): quasi-nucleons
Hierarchy of nuclear degrees of freedom

Reductive and Emergent
\[ \Rightarrow \text{EFT (see 2017 Saclay workshop)} \]

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Where does EDF/DFT fit in?
[Universal] nuclear energy functional phenomenologies

- **Nonrelativistic [HFB] functionals**
  - Skyrme — local densities and $\nabla s$
  - Gogny — finite range Gaussians
  - Fayans — self-consistent FFS

- **Relativistic [covariant Hartree + pairing = RHB] functionals**
  - RMF — meson fields (generalized Walecka model)
  - point coupling Lagrangian

1. Repeat cycle until stops changing (self-consistent):
   - densities $\rho_i \rightarrow$ potential that minimizes energy $E[\rho_i] \rightarrow$ s.p. states $\rightarrow \rho_i$
   - Densities (or density matrices) from single-particle wave functions
   - Includes pairing densities, i.e., $\langle \psi_i \psi_j \rangle$ as well as $\langle \psi_i^\dagger \psi_j \rangle$

2. [Restore symmetries, beyond-mean-field correlations (or SR $\rightarrow$ MR)]

3. Evaluate observables (masses, radii, $\beta$-decay, fission . . . )

Often interpreted as Kohn-Sham density functional theory
Motivations for doing better than empirical EDFs

- Apparent model dependence (systematic errors?)
- Extrapolations to driplines, large $A$, high density are uncontrolled
- Breakdown and failure mode is unclear: e.g., should EDFs work to the driplines?
- More accuracy wanted for $r$-process: is this even possible?
- What observables? Coupling to external currents? $0\nu\beta\beta$ m.e.?
- Connect to nuclear EFTs (and so to QCD)

...
Emergent features of nuclear energy density functionals

- Precise liquid drop systematics
- Shell structure
- Superfluidity
- Low-lying collectivity (RPA)

- Naturalness of parameter values reflect underlying chiral physics
- But SVD analyses reveal hierarchy of physics
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Naturalness of parameter values reflect underlying chiral physics

But SVD analyses reveal hierarchy of physics

- Multiple studies show relatively few important parameters and they reflect emergent properties
- Recent: Bulgac et al., “A Minimal Nuclear Energy Density Functional”

See also Toivanen et al., PRC (2008)
Fine-tuned potentials based on chiral EFT [from G. Hagen]

Accurate BEs from light $\rightarrow$ heavy $\rightarrow$ infinite matter from a chiral interaction

- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate

1.8/2.0 (EM) from K. Hebeler et al PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)
What is the take-away message from phenomenological success? How far can we push this approach? How does it relate to EDF/DFT?
General questions for phenomenological EDFs

- Are density dependencies too simplistic? How do you know?
- How should we organize possible terms in the EDF?
- Where is pion physics resolved? Does near-unitarity matter?
- What is the connection to many-body forces?
- How do we estimate \textit{a priori} theoretical uncertainties?
- What is the theoretical limit of accuracy?
- and so on ...

⇒ Extend or modify EDF forms in (semi-)controlled way
⇒ Use microscopic many-body theory for guidance

There are multiple paths to a nuclear EDF ⇒ What about EFT?
Some current strategies for nuclear EDFs guided by EFT

Extend or modify conventional EDF forms in (semi-)controlled ways

1. Long-distance chiral physics from Weinberg PC expansion
   - Density matrix expansion (DME) applied to NN and NNN diagrams
   - [Re-fit residual Skyrme parameters and test description]
   - MBPT expansion justified by phase-space-based power counting

2. In-medium chiral perturbation theory [Munich group]
   - ChPT loop expansion becomes EOS expansion
   - Apply DME to get DFT functional

3. Extend existing functionals following EFT principles
   - Non-local regularized pseudo-potential [Raimondi et al., 1402.1556]
   - Optimize pseudo-potential to experimental data and test
   - [See also J. Dobaczewski arXiv:1507.00697 for ab initio → EDF]

4. RG evolution of effective action functional [Jens Braun et al.]
   - See H. Liang et al. [arXiv:1710.00650] for recent implementation

Can we develop bottom-up EFT for DFT using a QFT formulation?
[See expansion about unitary limit in talks at Orsay workshop!]
Outline

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Extra: Statistical tools and recent RKE potentials
Long-range parts of chiral expansion with and without $\Delta$s

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<th></th>
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<td>$\Delta$-less EFT</td>
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<tr>
<td><strong>LO</strong></td>
<td><img src="image1" alt="Graph" /></td>
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Microscopically constrained EDF
Implementing Chiral Interactions in DFT

- Hartree-Fock fields from Chiral interactions
  - Skyrme + Gaussian Hartree + DME Fock

  UNEDF2 like and refitted to masses and radii
  Chiral and fixed for a given order, LECs and regulator

- Start with a ‘conservative’ regulator, $r_c = 2.0$ fm

- Refit skyrme parameters

- Move to a ‘less conservative’ regulator

- Rinse and repeat

Study the effect of the regulator and rise of finite size effects
Non-local densities when working with finite range potentials

\[ V_{NN}^H \sim \int dR \, dr \, \langle r | V_{NN} | r \rangle \rho_1(R + \frac{r}{2}) \rho_2(R - \frac{r}{2}) \]

\[ V_{NN}^F \sim \int dR \, dr \, \langle r | V_{NN} | r \rangle \rho_1(R - \frac{r}{2}, R + \frac{r}{2}) \rho_2(R + \frac{r}{2}, R - \frac{r}{2}) P_{12} \]

Density Matrix Expansion

\[ \rho(R + \frac{r}{2}, R - \frac{r}{2}) \approx \Pi_0^\rho(k_F r) \rho(R) + \frac{r^2}{6} \Pi_2^\rho(k_F r) \left[ \frac{1}{4} \Delta \rho(R) - \tau(R) + \frac{3}{5} k_F^2 \rho(R) \right] \]

Density dependent couplings enter in the Fock Energy
Microscopically constrained EDF
Finite Range Chiral Potentials

- Chiral potentials are regulated

\[ V_c(r) \propto \left[ 1 - e^{-r^2/r^2_c} \right]^n e^{-2x/r^6} \ldots \]

- Expand as a sum of Gaussians

\[ V_G(r) = \sum_{i=1}^{N-1} V_i \left( e^{-\mu_i r^2} - e^{-\mu_N r^2} \right) \]

Allows to use the already implemented Gogny machinery
Microscopically constrained EDF
Density Dependent Couplings

- Expensive numerical integrals

\[ g_t^{\rho \rho}(\rho) \propto \int dr \ r^2 \left[ \left[ \Pi_0^\rho (k_F r) \right]^2 + \ldots \right] \left[ V_c(r) + 3W_c(r) + \ldots \right] \]

- Interpolating function

\[ g_t^{\rho \rho}(\rho) = g_0 + \sum_{i=1}^{M} a_i \left[ \tan^{-1} (b_i \rho^{c_i}) \right] \]

- The same for 3N forces

Derivatives with respect of \( \rho \) are available
Microscopically constrained EDF
Density Dependent Couplings

- Expensive numerical integrals
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Derivatives with respect of \( \rho \) are available
Microscopically constrained EDF
Infinite Nuclear Matter Properties

- Used to constrain the Skyrme phenomenological parameters

- Energy density in nuclear matter

\[
W(\rho_0) = \left[ C_0^\rho + g_0^\rho(\rho_0) + \rho_0 h_0^\rho(\rho_0) \right] \rho_0 \\
+ \left[ C_0^{\rho\tau} + g_0^{\rho\tau}(\rho_0) + \rho_0 h_0^{\rho\tau}(\rho_0) \right] \tau_0 + W_{FR}(\rho_0)
\]

- Taylor expansion around saturation density

\[
W(\rho_0) = \frac{E_{NM}}{A} + \frac{P_{NM}}{\rho_c^2}(\rho_0 - \rho_c) + \frac{K_{NM}}{18 \rho_c^2}(\rho_0 - \rho_c)^2 + \cdots
\]

- Calculate derivatives of \( W(\rho_0) \) and solve for \( C_0^{\rho\rho}, C_0^{\rho\tau}, C_1^{\rho\rho}, C_1^{\rho\tau}, \ldots \)

Use NMP as inputs to obtain Skyrme couplings
Preliminary results: Mass residuals (single reference)

Root mean square deviations between experimental and theoretical binding energies (in MeV). Experimental values are taken from the 2016 Atomic Mass Evaluation.

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Preliminary results: Mass residuals (single reference)

Look at pattern of residuals as a function of $N$ ...

What can conclude from this? Is MR necessary to judge DME?
Cf. effect on Gogny HFB mass residuals of (some) BMF

\[ V(1, 2) = \sum_{j=1,2} e^{-\frac{(r_1-r_2)^2}{\mu_j^2}} \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right) \{ \mu_j \} = \{0.5, 1.0\} \text{ fm} \]

\[ + t_0 (1 + x_0 P_\sigma) \delta(r_1 - r_2) \rho(\mathbf{r})^\alpha + i W_{LS} \nabla_{12} \delta(r_1 - r_2) \times \nabla_{12} \cdot (\mathbf{\sigma}_1 + \mathbf{\sigma}_2) \]

- \approx 14 parameters
- quadrupole correlations included self-consistently
- D1M: \( \delta B_{\text{rms}} = 0.8 \text{ MeV} \) for 2353 masses
- \( \sigma \approx 0.65 \text{ MeV} \) for 2064 \( \beta \)-decay energies
- radii, giant resonances and fission properties
- does not include particle-vibration coupling

Clearly we need to include beyond-mean-field physics to fully address EDF needs!
DME: going forward

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- Test systematics along isotope chains. E.g., role of $2\pi$ 3NF

[Old calculations from Hergert et al., Cipollone et al. (2013). Now also SCGF and AFDMC!]
DME: going forward

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[Old calculations from Hergert et al., Cipollone et al. (2013). Now also SCGF and AFDMC!]

\[
\begin{align*}
E_{3,\text{Max}} & = 14 \\
\lambda & = 1.88 \text{ fm}^{-1}
\end{align*}
\]
Clearly we need to include beyond-mean-field physics to fully address EDF needs!

Test systematics along isotope chains. E.g., role of $2\pi$ 3NF

Beyond HF in DME $\Rightarrow$ are higher orders resolved?

- Cf. local counterterms for $T$-matrix contributions above cutoff $\Lambda$ (here: $\Lambda \rightarrow k_F$)
- Y. Zhang (OSU): Higher-order G-matrix well represented by gradient terms up to $\nabla^4$ near $k_{F\text{sat}}$
Outline

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How to proceed with EFT for DFT (or alternative)?

Extra: Statistical tools and recent RKE potentials
Many questions to address about EFT for DFT (or ?)
[see Drut, rjf, Platter, arXiv:0906.1463]

- What are the relevant degrees of freedom? Symmetries? [Can we have quasiparticles in the bulk?]
- Power counting: what is our expansion? Breakdown scale?
- Is there an RG argument to apply? (cf. scale toward Fermi surface)
- How should the EFT be formulated? Effective action? How do I think about parameterizing a density functional?
- How can we implement/expand about liquid drop physics?
- How do we reconcile the different EDF representations?
- Dealing with zero modes — can we adapt methods for gauge theories (for constraints)? What about collective surface vibrations?
- Can we implement such an EFT without losing the favorable computational scaling of current nuclear EDFs?
Effective actions and broken symmetries

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization $M$ in a spin system
  - introduce an **external field** $H$ to break rotational symmetry

if $F[H]$ calculated perturbatively, $M[H = 0] = 0$ to all orders
Effective actions and broken symmetries

- Natural framework for spontaneous symmetry breaking
  - e.g., test for zero-field magnetization $M$ in a spin system
  - introduce an external field $H$ to break rotational symmetry

- if $F[H]$ calculated perturbatively, $M[H = 0] = 0$ to all orders
- Legendre transform Helmholtz free energy $F(H)$:
  \[
  \text{invert } M = -\frac{\partial F(H)}{\partial H} \quad \Gamma[M] = F[H(M)] + MH(M)
  \]
  - since $H = \frac{\partial \Gamma}{\partial M} \rightarrow 0$, stationary points of $\Gamma \implies$ ground state
- Can couple source “$H$” many ways (and multiple sources)
DFT and effective actions (Fukuda et al., Polonyi, ...)  

- **External field** ↔ **Magnetization**
- Helmholtz free energy $F[H] \iff$ Gibbs free energy $\Gamma[M]$  

**Legendre transform**  

\[ \Gamma[M] = F[H] + H M \]  

\[ H = \frac{\partial \Gamma[M]}{\partial M} \quad \text{ground state} \quad \frac{\partial \Gamma[M]}{\partial M} \bigg|_{M_{gs}} = 0 \]
DFT and effective actions (Fukuda et al., Polonyi,...)

- External field $\iff$ Magnetization
- Helmholtz free energy $F[H] \iff$ Gibbs free energy $\Gamma[M]$

Legendre transform $\implies \Gamma[M] = F[H] + H M$

$H = \frac{\partial \Gamma[M]}{\partial M} \bigg|_{\text{state}} \div \frac{\partial \Gamma[M]}{\partial M} \bigg|_{M_{gs}} = 0$

- Partition function with sources $J$ that adjust (any) densities:
  \[ Z[J] = e^{-W[J]} \sim \text{Tr} e^{-\beta(\hat{H} + J \hat{\rho})} \implies \text{e.g., path integral for } W[J] \]

- Invert to find $J[\rho]$ and Legendre transform from $J$ to $\rho$:
  \[ \rho(x) = \frac{\delta W[J]}{\delta J(x)} \implies \Gamma[\rho] = W[J] - \int J \rho \quad \text{and} \quad J(x) = -\frac{\delta \Gamma[\rho]}{\delta \rho(x)} \]

$\implies \Gamma[\rho] \propto$ energy functional $E[\rho]$, stationary at $\rho_{gs}(x)$!
Pairing in Kohn-Sham DFT  [rjf, Hammer, Puglia, nucl-th/0612086]

- Add source $j$ coupled to anomalous density:

$$Z[J, j] = e^{-W[J,j]} = \int D(\psi^\dagger \psi) \exp\left\{ -\int dx \left[ \mathcal{L} + J(x) \psi_\alpha^\dagger \psi_\alpha + j(x)(\psi_\uparrow^\dagger \psi_\downarrow^\dagger + \psi_\downarrow \psi_\uparrow) \right] \right\}$$

- Densities found by functional derivatives wrt $J, j$:

$$\rho(x) = \frac{\delta W[J, j]}{\delta J(x)} \bigg|_j, \quad \phi(x) \equiv \langle \psi^\dagger_\uparrow(x) \psi^\dagger_\downarrow(x) + \psi_\downarrow(x) \psi^\dagger_\uparrow(x) \rangle_{J,j} = \frac{\delta W[J, j]}{\delta j(x)} \bigg|_J$$

- Find $\Gamma[\rho, \phi]$ from $W[J_0, j_0]$ by inversion  ($\Delta = \Delta_0 + \Delta_1 + \cdots$)

- Kohn-Sham system $\rightarrow$ short-range HFB with $j_0$ as gap

$$\begin{pmatrix} h_0(x) - \mu_0 & j_0(x) \\ j_0(x) & -h_0(x) + \mu_0 \end{pmatrix} \begin{pmatrix} u_i(x) \\ v_i(x) \end{pmatrix} = E_i \begin{pmatrix} u_i(x) \\ v_i(x) \end{pmatrix}$$

where  

$$h_0(x) \equiv -\frac{\nabla^2}{2M} + J_0(x)$$

- New renormalization counterterms needed (e.g., $\frac{1}{2} \zeta j^2$)
Pairing in Kohn-Sham DFT  

- Add source \( j \) coupled to anomalous density:

\[
Z[J,j] = e^{-W[J,j]} = \int D(\psi^\dagger \psi) \exp \left\{ -\int dx \left[ \mathcal{L} + J(x) \psi_\alpha^\dagger \psi_\alpha + j(x)(\psi_\uparrow^\dagger \psi_\downarrow^\dagger + \psi_\downarrow \psi_\uparrow) \right] \right\}
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- Kohn-Sham system \( \Rightarrow \) short-range HFB with \( j_0 \) as gap

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\]

where \( h_0(x) \equiv -\frac{\nabla^2}{2M} + J_0(x) \)

- New renormalization counterterms needed (e.g., \( \frac{1}{2} \zeta \jmath^2 \))

In general: adding more sources improves variational probing and KS Green’s function gets closer to full Green’s function (see old refs)
But there are different effective action formulations

- Couple source to local Lagrangian field, e.g., $J(x)\phi(x)$
  - $\Gamma[\varphi]$ where $\varphi(x) = \langle \phi(x) \rangle \implies$ 1PI effective action
  - Arises from fermion $\mathcal{L}$’s by introducing auxiliary (HS) fields
  - See nucl-th/0208058 for dilute EFT in large $N \implies$ loop expansion

- Couple $J$ to non-local composite op, e.g., $J(x, x')\phi(x)\phi(x')$
  - $\Gamma[G, \varphi] \implies$ 2PI effective action [CJT]
  - Cf. Baym-Kadanoff conserving ("$\Phi$-derivable") approximations
  - Cf. self-consistent Green’s functions or RG-evolved effective action

- Source coupled to local composite operator, e.g., $J(x)\phi^2(x)$
  - 2PPI (two-particle-point-irreducible) effective action
  - Kohn-Sham DFT from order-by-order inversion method
  - Careful: new divergences arise (e.g., pairing)
What would a condensed matter theorist do?

From Altland and Simons “Condensed Matter Field Theory”:

![Diagrams](image)

Figure 6.1 On the different channels of decoupling an interaction by Hubbard–Stratonovich transformation. (a) Decoupling in the “density” channel; (b) decoupling in the “pairing” or “Cooper” channel; and (c) decoupling in the “exchange” channel.

- May want to HS decouple in all three channels with \( q \ll |p_i| \):

\[
S_{\text{int}}[\overline{\psi}, \psi] \approx \frac{1}{2} \sum_{p, p', q} \left( \overline{\psi}_{\sigma p} \psi_{\sigma p + q} V(q) \overline{\psi}_{\sigma' p'} \psi_{\sigma' p' - q} - \overline{\psi}_{\sigma p} \psi_{\sigma' p + q} V(p' - p) \overline{\psi}_{\sigma' p' + q} \psi_{\sigma' p'} \right.
\]

- Or exploit freedom in saddlepoint evaluation [see Negele and Orland]
Nuclei are self-bound $\implies$ KS potentials break symmetries

- Conceptual issue: Is Kohn-Sham DFT well defined?
  - J. Engel: ground state density spread uniformly over space
  - Want DFT for *internal* densities

- Practical issue: what to do when KS potentials break symmetries?
  - Symmetry restoration with superposition of states:
    $$ |\psi\rangle = \int d\alpha f(\alpha)|\phi\rangle \implies \text{minimize wrt } f(\alpha), \text{ before or after } |\phi\rangle $$

  - Wave function method strategies for “center of mass” problem
    - isolate “internal” dofs, e.g., with Jacobi coordinates
    - work in HO Slater determinant basis for which COM decouples
    - work with internal Hamiltonian so that COM part factors

- How to accommodate within effective action DFT framework?
  - Zero-frequency modes $\implies$ divergent perturbation expansion
  - Transformation to collective variables $\implies$ work with overcomplete dof’s $\implies$ system with constraints
  - Can we apply methods for gauge theories?
Zero modes: collective coordinates and functional integrals

- See Zinn-Justin, Path Integrals in Quantum Mechanics
  - In general, introduce collective coordinates; if possible, switch
  - If not feasible, apply Faddeev-Popov’s method (cf. quantizing non-abelian gauge theories)

Another possible approach: use BRST invariance
Add more fermionic variables (ghosts) so more overcomplete
Apparent complication is actually a simplification because in gauge systems there is a supersymmetry
Examples in the literature with applications to mechanical systems
E.g., Bes and Kurchan, “The treatment of collective coordinates in many-body systems: An application of the BRST invariance”

Can the procedure be adapted to DFT?

Status report
Past progress: negligible :)
Current plan: revisiting for model problems; cautiously optimistic
Help would be welcome!
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Outline

Viewpoint: nuclear reduction and emergence

(Preliminary) results from new DME implementation

How to proceed with EFT for DFT (or alternative)?

Extra: Statistical tools and recent RKE potentials