Importance Truncated NCSM with Chiral NN plus 3N Interactions

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Nuclear Structure

From QCD to Nuclear Structure

- chiral EFT based on the relevant degrees of freedom & symmetries of QCD
- provides consistent NN & 3N interaction plus currents
- in the following:
  - NN at N^3LO (Entem & Machleidt, 500 MeV)
  - 3N at N^2LO (low-energy constants c_D & c_E from triton fit)

Low-Energy QCD

NN+3N Interaction from Chiral EFT
Nuclear Structure

Unitarily Transformed Hamiltonian

- adapt Hamiltonian to truncated low-energy model space
  - tame short-range correlations
  - improve convergence behavior
- transform Hamiltonian & observables consistently
- conserve experimentally constrained few-body properties

NN+3N Interaction from Chiral EFT

Low-Energy QCD
From QCD to Nuclear Structure

Nuclear Structure

Exact & Approx. Many-Body Methods

Unitarily Transformed Hamiltonian

NN+3N Interaction from Chiral EFT

Low-Energy QCD

- ‘exact’ solution of the many-body problem for light & intermediate masses (NCSM, CC, ...)
- controlled approximations for heavier nuclei (HF & MBPT, ...)
- all rely on restricted model spaces & benefit from unitary transformation
From QCD to Nuclear Structure

Nuclear Structure

- Exact & Approx. Many-Body Methods
- Unitarily Transformed Hamiltonian
- NN+3N Interaction from Chiral EFT

Low-Energy QCD

focus on consistent inclusion of chiral 3N interaction
Overview

- Unitarily Transformed NN+3N Hamiltonians
  - Similarity Renormalization Group
  - consistent transformation of chiral NN+3N interactions

- Exact Ab-Initio Calculations
  - Importance-Truncated NCSM
  - test of SRG-transformed chiral NN+3N interactions throughout the p-shell

- Approximate Many-Body Methods
  - Hartree-Fock & Perturbation Theory
  - ground-state systematics throughout the nuclear chart using SRG-transformed chiral NN+3N interactions
Unitarily Transformed Hamiltonians

Similarity Renormalization Group

Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
evolution of the Hamiltonian to band-diagonal form with respect to uncorrelated many-body basis

**unitary transformation** of Hamiltonian:

\[ \tilde{H}_\alpha = U_\alpha^\dagger H U_\alpha \]

**evolution equations** for \( \tilde{H}_\alpha \) and \( U_\alpha \) depending on generator \( \eta_\alpha \):

\[ \frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \]
\[ \frac{d}{d\alpha} U_\alpha = -U_\alpha \eta_\alpha \]

**dynamic generator**: commutator with the operator in whose eigenbasis \( H \) shall be diagonalized

\[ \eta_\alpha = (2\mu)^2[T_{\text{int}}, \tilde{H}_\alpha] \]
represent operator equation in \textit{n-body Jacobi HO basis} \( |EiJ^\pi T\rangle \)

- \( n = 2 \): relative LS-coupled HO states: \( |E(\text{LS})J^\pi T\rangle \)
- \( n = 3 \): antisymmetrized Jacobi-coordinate HO states: \( |EiJ^\pi T\rangle \)

system of \textit{coupled evolution equations} for each \((J^\pi T)\)-block

\[
\frac{d}{d\alpha} \langle EiJ^\pi T | \tilde{H}_\alpha | E'iJ^\pi T \rangle = (2\mu)^2 \sum_{E'',i''} \sum_{E''',i'''} \Bigg[ \\
\langle EiJ^\pi T | T_{\text{int}} | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E''''i''''J^\pi T \rangle \langle E''''i''''J^\pi T | \tilde{H}_\alpha | E'iJ^\pi T \rangle \\
- 2 \langle EiJ^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | T_{\text{int}} | E''''i''''J^\pi T \rangle \langle E''''i''''J^\pi T | \tilde{H}_\alpha | E'iJ^\pi T \rangle \\
+ \langle EiJ^\pi T | \tilde{H}_\alpha | E''i''J^\pi T \rangle \langle E''i''J^\pi T | \tilde{H}_\alpha | E''''i''''J^\pi T \rangle \langle E''''i''''J^\pi T | T_{\text{int}} | E'iJ^\pi T \rangle \Bigg]
\]

we use \( E_{\text{SRG}} = 40 \) for \( J \leq 5/2 \) and ramp down to 24 in steps of 4 (sufficient to converge the intermediate sums for \( \hbar\Omega \gtrsim 16 \text{ MeV} \))
SRG Evolution in Two-Body Space

\[ \alpha = 0.00 \text{ fm}^4 \]

\[ \Lambda = \infty \text{ fm}^{-1} \]

\[ J^{\pi} = 1^+, T = 0, \hbar \Omega = 28 \text{ MeV} \]

2B-Jacobi HO matrix elements

momentum space \( ^3S_1 \)
SRG Evolution in Two-Body Space

\[ \alpha = 0.32 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ J^\pi = 1^+, T = 0, \hbar \Omega = 28 \text{ MeV} \]

2B-Jacobi HO matrix elements

momenum space \[^3S_1\]
SRG Evolution in Three-Body Space

$\alpha = 0.00 \text{ fm}^4$

$\Lambda = \infty \text{ fm}^{-1}$

$J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 28 \text{ MeV}$

3B-Jacobi HO matrix elements

NCSM ground state $^3\text{H}$
\[ \alpha = 0.32 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ J^{\pi} = \frac{1}{2}^+, T = \frac{1}{2}, \hbar\Omega = 28 \text{ MeV} \]

NCSM ground state \(^3\text{H}\)
Calculations in A-Body Space

- **cluster decomposition**: decompose evolved Hamiltonian from 2B/3B space into irreducible $n$-body contributions $\tilde{H}_\alpha^{[n]}$

  $$\tilde{H}_\alpha = \tilde{H}_\alpha^{[1]} + \tilde{H}_\alpha^{[2]} + \tilde{H}_\alpha^{[3]} + \ldots$$

- **cluster truncation**: can construct cluster-orders up to $n = 3$ from evolution in 2B and 3B space, have to discard $n > 3$

  - only the **full evolution in A-body space** conserves A-body energy eigenvalues and, thus, independent of $\alpha$

  - $\alpha$-dependence of eigenvalues of cluster-truncated Hamiltonian measures impact of omitted many-body interactions

  $\alpha$-variation provides a **diagnostic tool** to assess the contributions of omitted many-body interactions
Sounds easy, but...

1. **computation of initial 2B/3B-Jacobi HO matrix elements of chiral NN+3N interactions**
   - we use Petr Navratil’s ManyEff code for computing 3B-Jacobi matrix elements and corresponding CFPs

2. **SRG evolution in 2B/3B space and cluster decomposition**
   - efficient implementation using adaptive ODE solver; largest block takes a few hours on single node

3. **transformation of 2B/3B Jacobi HO matrix elements into JT-coupled representation**
   - formulated transformation directly into JT-coupled scheme; highly efficient implementation; can handle $E_{3\text{max}} = 16$ in JT-coupled scheme

4. **data management and on-the-fly decoupling in many-body codes**
   - invented optimized storage scheme for fast on-the-fly decoupling; can keep all matrix elements up to $E_{3\text{max}} = 16$ in memory
Exact Ab-Initio Calculations

Importance Truncated NCSM

Importance Truncated NCSM

- converged NCSM calculations essentially restricted to lower/mid p-shell
- full 10 or 12ℏΩ calculation for $^{16}\text{O}$ hardly feasible (basis dimension $> 10^{10}$)

Importance Truncation
reduce NCSM space to the relevant basis states using an \textit{a priori} importance measure derived from MBPT
Importance Truncation: Basic Idea

- given a initial approximation $|\psi_{\text{ref}}\rangle$ for the target state within a limited reference space $\mathcal{M}_{\text{ref}}$

  $|\psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C^{(\text{ref})}_{\nu} |\Phi_{\nu}\rangle$

- measure the importance of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

  $\kappa_{\nu} = -\left\langle \Phi_{\nu} | H_{\text{int}} | \psi_{\text{ref}} \right\rangle$

  importance measure only probes 2p2h excitations on top of $\mathcal{M}_{\text{ref}}$ for a two-body Hamiltonian

- construct importance-truncated space $\mathcal{M}(\kappa_{\text{min}})$ spanned by basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

- solve eigenvalue problem in $\mathcal{M}(\kappa_{\text{min}})$ and obtain improved approximation of target state

  embed into iterative scheme to access full model space
Importance Truncation: Iterative Schemes

**IT-NCSM(i) or IT-CI(i)**

- simple iterative scheme for arbitrary model spaces
- ✧ start with $|\psi_{\text{ref}}\rangle = |\Phi_0\rangle$
- ① construct importance truncated space containing up to $2p^2\hbar$ on top of $|\psi_{\text{ref}}\rangle$
- ② solve eigenvalue problem
- ③ use components of eigenstate with $|C_\nu| \geq C_{\text{min}}$ as new $|\psi_{\text{ref}}\rangle$
- ④ goto ① (until convergence)

**IT-NCSM(seq)**

- sequential update scheme for a set of $N_{\text{max}}\hbar\Omega$ spaces
- ✧ start with full NCSM eigenstate for small $N_{\text{max}}$ as initial $|\psi_{\text{ref}}\rangle$
- ① construct importance truncated space for $N_{\text{max}} + 2$
- ② solve eigenvalue problem
- ③ use components of eigenstate with $|C_\nu| \geq C_{\text{min}}$ as new $|\psi_{\text{ref}}\rangle$
- ④ goto ①

**Full NCSM space is recovered** in the limit $(\kappa_{\text{min}}, C_{\text{min}}) \to 0$
Threshold Extrapolation

- do calculations for a sequence of importance thresholds $\kappa_{\text{min}}$
- observables show smooth threshold dependence
- systematic approach to the full NCSM limit
- use a posteriori extrapolation $\kappa_{\text{min}} \to 0$ of observables to account for effect of excluded configurations
Constrained Threshold Extrapolation

\[ ^{16}\text{O}, \text{IT-NCSM(seq)} \]
\[ \text{S-SRG(CDB2k), } \hbar \Omega = 24 \text{ MeV, } N_{\text{max}} = 12 \]

- estimate energy contribution of excluded states perturbatively → \( \Delta_{\text{excl}}(\kappa_{\text{min}}) \)

- **simultaneous fit** of combined energy

\[
E_{\lambda}(\kappa_{\text{min}}) = E_{\text{int}}(\kappa_{\text{min}}) + \lambda \Delta_{\text{excl}}(\kappa_{\text{min}})
\]

for set of \( \lambda \)-values with the constraint \( E_{\lambda}(0) = E_{\text{extrap}} \)

- **robust threshold extrapolation** with error bars determined by variation of fit function
Benchmarking SRG-Evolved Chiral NN+3N Hamiltonians
A Tale of Three Hamiltonians

- **NN only**: start with NN-only initial Hamiltonian and evolve in two-body space

\[ \tilde{H}^{\text{NN-only}}_{\alpha} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int, } \alpha} + \tilde{V}^{[2]}_{\text{NN}, \alpha} \]

- **NN+3N-induced**: start with NN-only initial Hamiltonian and evolve in three-body space

\[ \tilde{H}^{\text{NN+3N-induced}}_{\alpha} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int, } \alpha} + \tilde{V}^{[2]}_{\text{NN}, \alpha} + \tilde{T}^{[3]}_{\text{int, } \alpha} + \tilde{V}^{[3]}_{\text{NN}, \alpha} \]

- **NN+3N-full**: start with NN+3N initial Hamiltonian and evolve in three-body space

\[ \tilde{H}^{\text{NN+3N-full}}_{\alpha} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int, } \alpha} + \tilde{V}^{[2]}_{\text{NN}, \alpha} + \tilde{T}^{[3]}_{\text{int, } \alpha} + \tilde{V}^{[3]}_{\text{NN}, \alpha} \]

α-variation provides a diagnostic tool to assess the contributions of omitted many-body interactions.
\(^4\text{He}: \text{Ground-State Energies}\)

- **NN only**
  - strong \(\alpha\)-dependence: induced 3N interactions
  - \(\hbar\Omega = 20 \text{ MeV}\)

- **NN+3N-induced**
  - no \(\alpha\)-dependence: no induced 4N interactions

- **NN+3N-full**
  - no \(\alpha\)-dependence: no induced 4N interactions

\[\begin{align*}
\alpha &= 0.04 \text{ fm}^4 & \alpha &= 0.05 \text{ fm}^4 & \alpha &= 0.0625 \text{ fm}^4 & \alpha &= 0.08 \text{ fm}^4 & \alpha &= 0.16 \text{ fm}^4 \\
\Lambda &= 2.24 \text{ fm}^{-1} & \Lambda &= 2.11 \text{ fm}^{-1} & \Lambda &= 2.00 \text{ fm}^{-1} & \Lambda &= 1.88 \text{ fm}^{-1} & \Lambda &= 1.58 \text{ fm}^{-1}
\end{align*}\]
\[\hbar \Omega = 20 \text{ MeV}\]

**NN only**

\[E = -22, -24, -26, -28, -30, -32, -34\] MeV

\[N_{\text{max}} = 2, 4, 6, 8, 10, 12, 14\]

\[\alpha = 0.04 \text{ fm}^4, \quad \Lambda = 2.24 \text{ fm}^{-1}\]

**NN+3N-induced**

\[E = -22, -24, -26, -28, -30, -32, -34\] MeV

\[N_{\text{max}} = 2, 4, 6, 8, 10, 12, 14\]

\[\alpha = 0.05 \text{ fm}^4, \quad \Lambda = 2.11 \text{ fm}^{-1}\]

**NN+3N-full**

\[E = -22, -24, -26, -28, -30, -32, -34\] MeV

\[N_{\text{max}} = 2, 4, 6, 8, 10, 12, 14\]

\[\alpha = 0.0625 \text{ fm}^4, \quad \Lambda = 2.00 \text{ fm}^{-1}\]
$^6\text{Li}$: Excitation Energies

### NN only

- $E_x$ vs $N_{\text{max}}$
- $\hbar \Omega = 20 \text{ MeV}$
- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$

### NN+3N-induced

- $E_x$ vs $N_{\text{max}}$
- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$

### NN+3N-full

- $E_x$ vs $N_{\text{max}}$
- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$
- $\Lambda = 1.88 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$
$^{12}\text{C}$: Ground-State Energies

**NN only**

- $\hbar \Omega = 20 \text{ MeV}$
- $N_{\text{max}}$
- $E$ [MeV]
- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$

**NN+3N-induced**

- no $\alpha$-dependence:
  - no induced 4N contrib.

**NN+3N-full**

- some $\alpha$-dependence:
  - induced 4N interactions

- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$
- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$
- $\alpha = 0.08 \text{ fm}^4$
- $\Lambda = 1.88 \text{ fm}^{-1}$
- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$
\( E_x \) [MeV]

\begin{align*}
\hbar \Omega &= 20 \text{ MeV} \\
N_{\text{max}}
\end{align*}

\[ \alpha = 0.04 \text{ fm}^4 \quad \Lambda = 2.24 \text{ fm}^{-1} \]
\[ \alpha = 0.05 \text{ fm}^4 \quad \Lambda = 2.11 \text{ fm}^{-1} \]
\[ \alpha = 0.0625 \text{ fm}^4 \quad \Lambda = 2.00 \text{ fm}^{-1} \]
\[ \alpha = 0.08 \text{ fm}^4 \quad \Lambda = 1.88 \text{ fm}^{-1} \]
\[ \alpha = 0.16 \text{ fm}^4 \quad \Lambda = 1.58 \text{ fm}^{-1} \]
16\textsuperscript{O}: Ground-State Energies

**NN only**

- \( \hbar \Omega = 20 \text{ MeV} \)
- \( N_{\text{max}} \) vs. \( E \) [MeV]

**NN+3N-induced**

- no \( \alpha \)-dependence: no induced 4N contrib.
- \( \alpha = 0.04 \text{ fm}^4 \)
- \( \Lambda = 2.24 \text{ fm}^{-1} \)

**NN+3N-full**

- sizable \( \alpha \)-dependence: induced 4N interactions
- \( \alpha = 0.05 \text{ fm}^4 \)
- \( \Lambda = 2.11 \text{ fm}^{-1} \)

\( \alpha = 0.0625 \text{ fm}^4 \)
\( \Lambda = 2.00 \text{ fm}^{-1} \)
\( \alpha = 0.08 \text{ fm}^4 \)
\( \Lambda = 1.88 \text{ fm}^{-1} \)
\( \alpha = 0.16 \text{ fm}^4 \)
\( \Lambda = 1.58 \text{ fm}^{-1} \)
\[16^O: \text{Energy vs. Flow Parameter}\]

- **NN only**: strong \(\alpha\)-dependence \(\Rightarrow\) significant induced 3N contributions

- **NN+3N-induced**: no \(\alpha\)-dependence \(\Rightarrow\) all relevant induced terms from initial NN captured at 3N level

- **NN+3N-full**: sizable \(\alpha\)-dependence \(\Rightarrow\) additional induced terms caused by initial 3N appear at 4N level
\[16\text{O} \; \text{&} \; ^4\text{He}: \text{Energy vs. Flow Parameter}\]

\[\hbar \Omega = 20 \text{ MeV}\]

\[\begin{align*}
\text{\(16\text{O}\)} & \quad \begin{array}{c}
\text{\(E_\infty\)} \quad [\text{MeV}]
\end{array} \\
\text{\(\alpha\)} \quad [\text{fm}^4] & \quad \begin{array}{c}
-110 \\
-120 \\
-130 \\
-140 \\
-150 \\
-160 \\
-170 \\
-180
\end{array}
\end{align*}\]

\[\begin{align*}
\text{\(4\text{He}\)} & \quad \begin{array}{c}
\text{\(E_\infty\)} \quad [\text{MeV}]
\end{array} \\
\text{\(\alpha\)} \quad [\text{fm}^4] & \quad \begin{array}{c}
-25 \\
-26 \\
-27 \\
-28 \\
-29
\end{array}
\end{align*}\]

\[\text{\(\bullet\)} \quad \text{NN only} \quad \text{\(\text{\(\bullet\)}\)} \quad \text{NN+3N-induced} \quad \text{\(\text{\(\Delta\)}\)} \quad \text{NN+3N-full}\]
Approximate Many-Body Methods

Hartree-Fock & Perturbation Theory

Roth, Neff, Feldmeier — Prog. Part. Nucl. Phys. 65, 50 (2010)
Hartree-Fock & Perturbation Theory

HF & PT provides information on the systematics of ground-state observables over a wide mass range

- solution of the HF equations with 3N interaction computationally simple
- second-order PT for energy with 3N interaction also straightforward
- all following results preliminary with some limitations, but none of them will change the conclusions
  - 3N matrix elements only up to $E_{3\text{max}} = 12$
  - fixed oscillator frequency $\hbar\Omega = 28$ MeV
  - second-order perturbative correction includes NN contribution only
Systematics: E/A and $R_{\text{ch}}$

$E/A$ [MeV]

$R_{\text{ch}}$ [fm]

NN-only

$\alpha = 0.02 \text{ fm}^4$

$\alpha = 0.04 \text{ fm}^4$

$\alpha = 0.08 \text{ fm}^4$

experiment

$e_{\text{max}} = 14$

$E_{3,\text{max}} = 12$

$\hbar\Omega = 28 \text{ MeV}$

Robert Roth – TU Darmstadt – 02/2011
Systematics: $E/A$ and $R_{\text{ch}}$

![Graph showing systematics for $E/A$ and $R_{\text{ch}}$](image)

- $E/A$ [MeV]
- $R_{\text{ch}}$ [fm]

- **NN-only**
- **HF+PT**
- **HF**

- $\alpha = 0.02 \text{ fm}^4$
- $\alpha = 0.04 \text{ fm}^4$
- $\alpha = 0.08 \text{ fm}^4$

- $e_{\text{max}} = 14$
- $E_{3,\text{max}} = 12$
- $\hbar\Omega = 28 \text{ MeV}$

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Systematics: E/A and $R_{\text{ch}}$

NN + 3N-induced

$E/A$ [MeV]

$R_{\text{ch}}$ [fm]

$\alpha = 0.02 \text{ fm}^4$

$\alpha = 0.04 \text{ fm}^4$

$\alpha = 0.08 \text{ fm}^4$

$e_{\text{max}} = 14$

$E_{3,\text{max}} = 12$

$\hbar \Omega = 28 \text{ MeV}$

Robert Roth – TU Darmstadt – 02/2011
Systematics: E/A and \( R_{\text{ch}} \)

\[ \begin{align*}
\alpha &= 0.02 \text{ fm}^4 \\
\alpha &= 0.04 \text{ fm}^4 \\
\alpha &= 0.08 \text{ fm}^4 \\
\end{align*} \]

\[ e_{\text{max}} = 14 \]
\[ E_{3,\text{max}} = 12 \]
\[ \hbar \Omega = 28 \text{ MeV} \]

\( \text{HF+PT} \)

\( \text{HF} \)
Systematics: E/A and R_{ch}

\[ E/A \text{[MeV]} \]

\[ R_{ch} \text{[fm]} \]

\begin{align*}
\alpha &= 0.02 \text{ fm}^4 \\
\alpha &= 0.04 \text{ fm}^4 \\
\alpha &= 0.08 \text{ fm}^4
\end{align*}

\[ e_{\text{max}} = 14 \]
\[ E_{3,\text{max}} = 12 \]
\[ \hbar \Omega = 28 \text{ MeV} \]
Systematics: E/A and R_{ch}

\begin{itemize}
  \item \textbf{HF+PT} \quad \text{strong } \alpha\text{-dependence: induced 4N contributions are sizable}
  \item \textbf{HF}
\end{itemize}

\begin{align*}
  e_{\text{max}} &= 14 \\
  E_{3,\text{max}} &= 12 \\
  \hbar \Omega &= 28 \text{ MeV}
\end{align*}
Conclusions
Conclusions

- ab initio nuclear structure calculations with consistently SRG-evolved chiral NN+3N interactions
  - consistent SRG evolution up to the 3N level
  - efficient transformation and management of JT-coupled 3N matrix elements
  - IT-NCSM with full 3N interactions up to \( N_{\text{max}} = 12 \) (14) for all p-shell nuclei (and lower sd-shell)

- indications that induced 4N contributions resulting from initial 3N interaction become significant beyond mid-p-shell

- use modified SRG generators to suppress induced 4N contributions from the outset

- many exciting applications ahead...
thanks to my group & my collaborators

  Institut für Kernphysik, TU Darmstadt

- **P. Navrátil**
  TRIUMF Vancouver, Canada

- **S. Quaglioni**
  Lawrence Livermore National Laboratory, USA

- **H. Hergert, P. Piecuch**
  Michigan State University, USA

- **C. Forssén**
  Chalmers University of Technology, Sweden

- **H. Feldmeier, T. Neff,**...
  Gesellschaft für Schwerionenforschung (GSI)