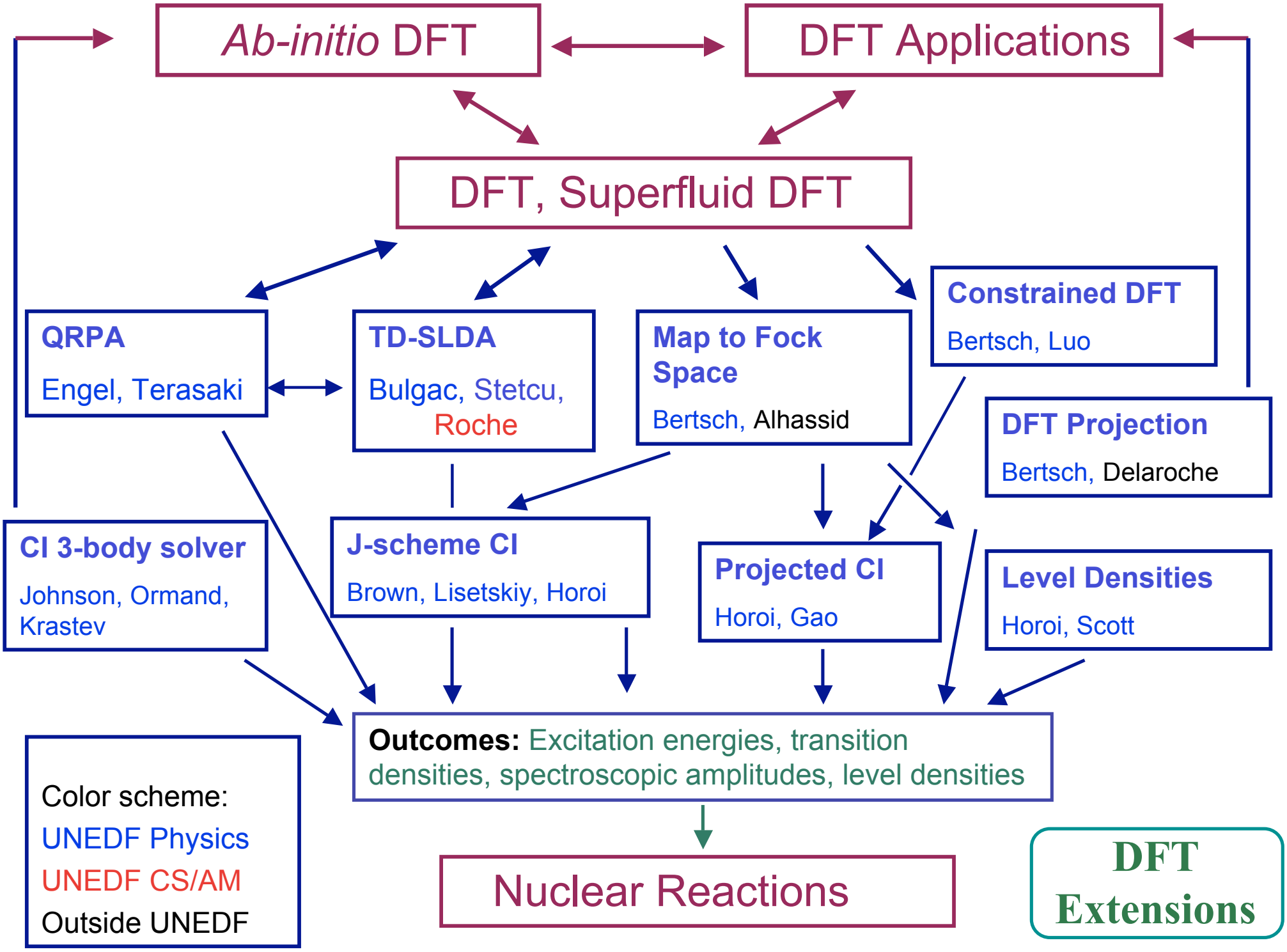
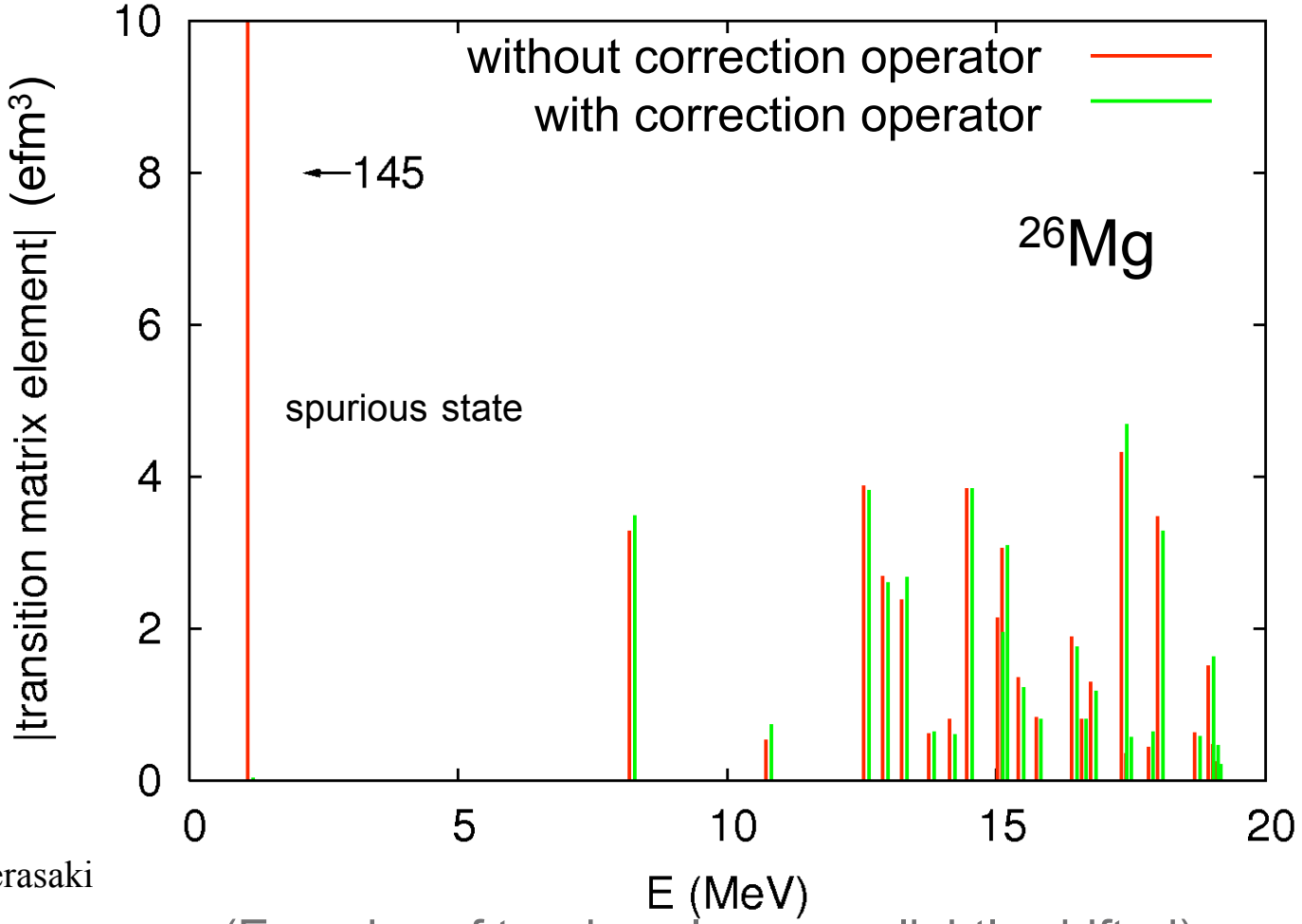

Ab-initio DFT
DFT Applications
DFT, Superfluid DFT
QRPA
Engel, Terasaki
TD-SLDA
Bulgac, Stetcu, Roche
Map to Fock Space
Bertsch, Alhassid
Constrained DFT
Bertsch, Luo
DFT Projection
Bertsch, Delaroche
CI 3-body solver
Johnson, Ormand, Krastev
J-scheme CI
Brown, Lisetskiy, Horoi
Projected CI
Horoi, Gao
Level Densities
Horoi, Scott
Outcomes: Excitation energies, transition densities, spectroscopic amplitudes, level densities
Nuclear Reactions
Color scheme:
UNEDF Physics
UNEDF CS/AM
Outside UNEDF
DFT Extensions

Year 3 Deliverables: Status, Work to be Done

- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - ✓ Use the deformed QRPA code to study low-lying collective states and weak decays: on track, major goals accomplished, study of the 2^+ states and resonances near the drip line remains to be done;
  - ✓ develop second-QRPA extension needed for reaction theory: formulation started, coding moved to year 5.
- **Bulgac, Stetcu, Magierski (UW), Roche (ORNL):**
  - ✓ Develop a coordinate representation Time-Dependent-DFT code TD-SLDA and apply it to excited states of nuclei: on track, major goals accomplished, extensive testing and applications remain to be done.
- **Horoi, Scott, Gao, Central Michigan Unversity:**
  - ✓ Use CI Moments code to calculate the nuclear level densities for the rp-process nuclei and provide input to Hauser-Feshbach treatment of reaction rates: on track, major goals accomplished, reaction cross sections remain to be calculated.
- **Brown, Lisetskiy, Michigan State University:**
  - ✓ Optimize performance of CI-NuShellX and speed it up by an order of magnitude: on track, to be finalized this summer.
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - ✓ Optimize performance and load-balance of CI-REDSTICK code with three-nucleon forces to reach 500M basis states in ^{12}C: on track, major goals accomplished, efficient 3-body Lanczos to be implemented by the end of Year 3 **(CS help needed).**

QRPA: Absolute value of transition matrix elements of $e\sum_{i=1}^{A} r_i^3 Y_{10}(\theta_i,\varphi_i)$ between ground and $K^\pi=0^-$ states

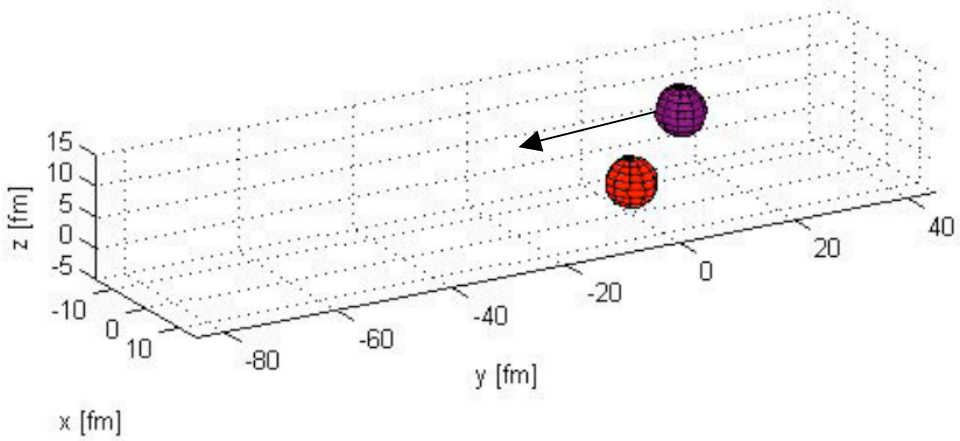
Difference between results with and without "correction operator" in excitations is measure of size of spurious components.

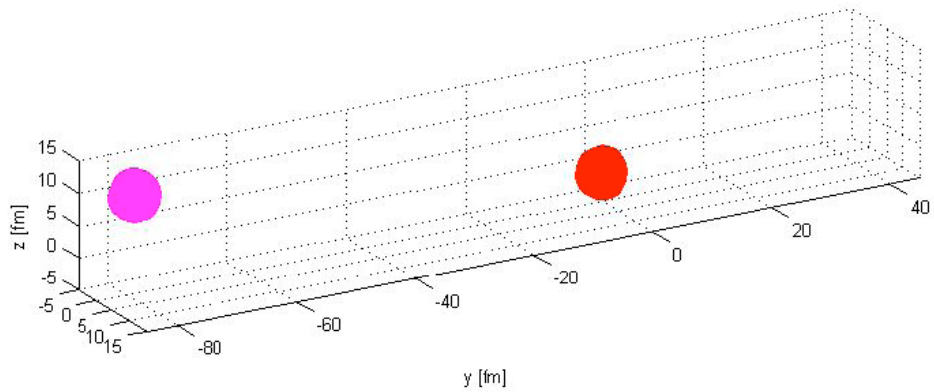


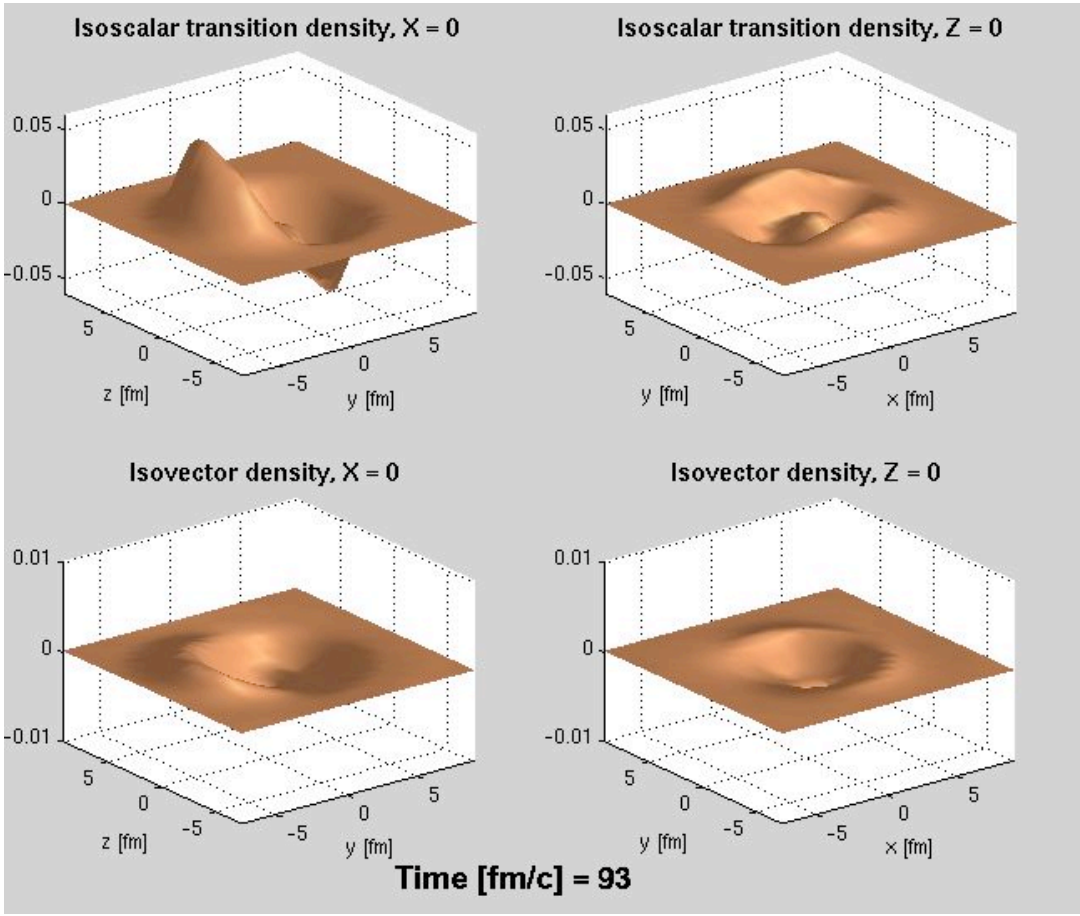
(Energies of two impulses are slightly shifted)

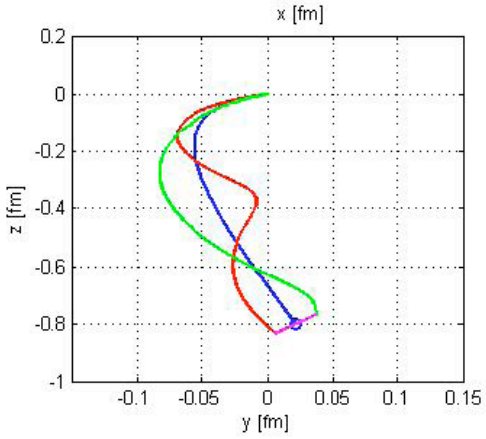
Prepared by J. Terasaki and J. Engel

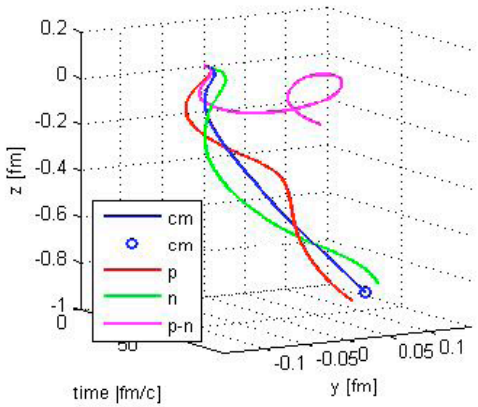
Bulgac, Stetcu, Magierski, Roche

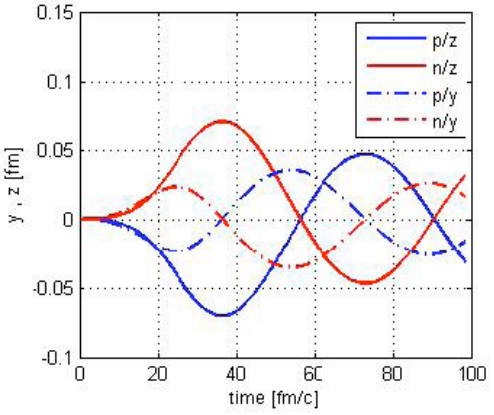




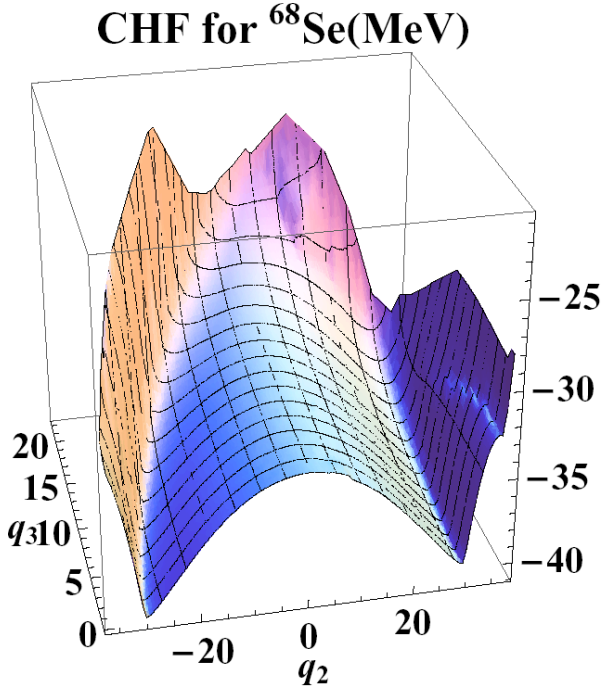




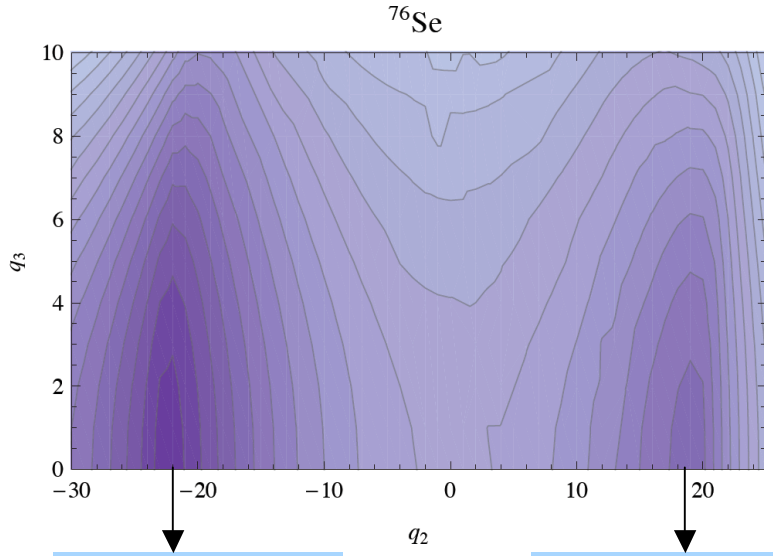


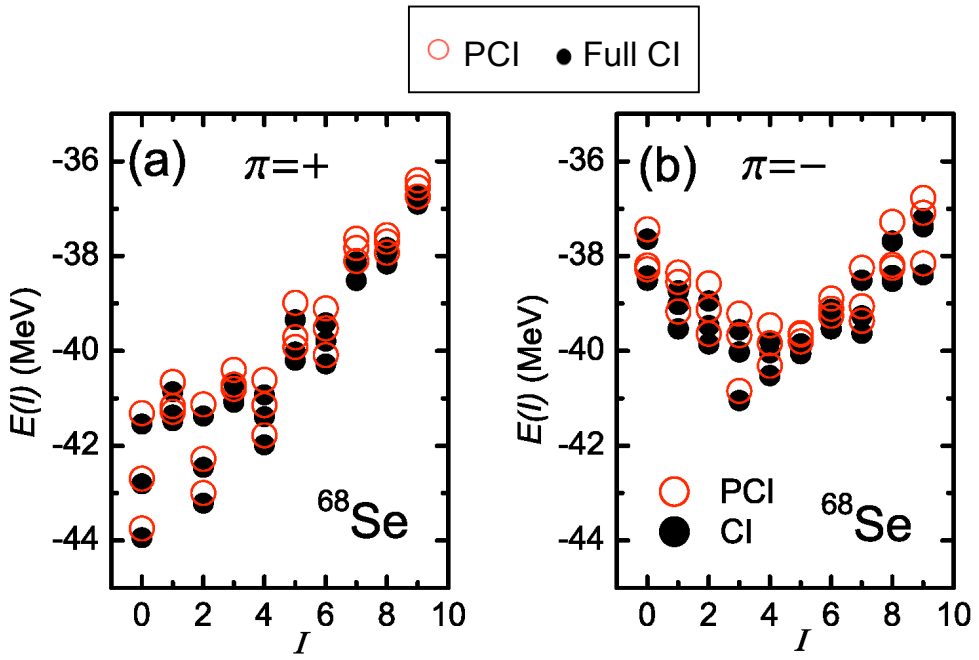


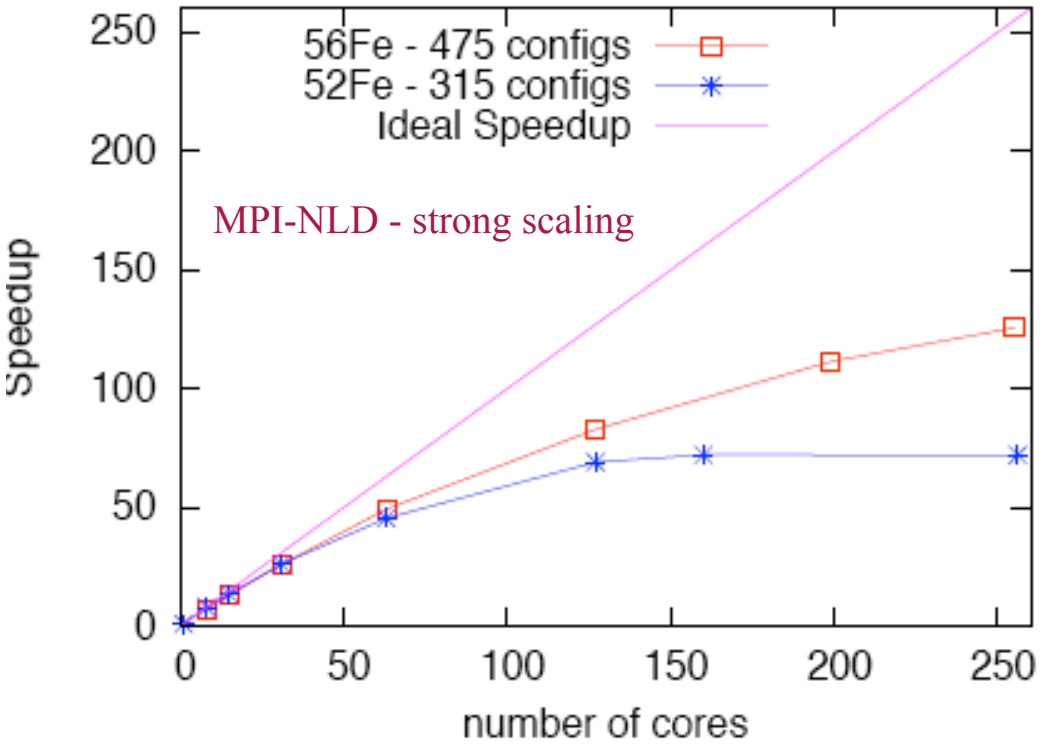
Parity Projected CI (PPCI)



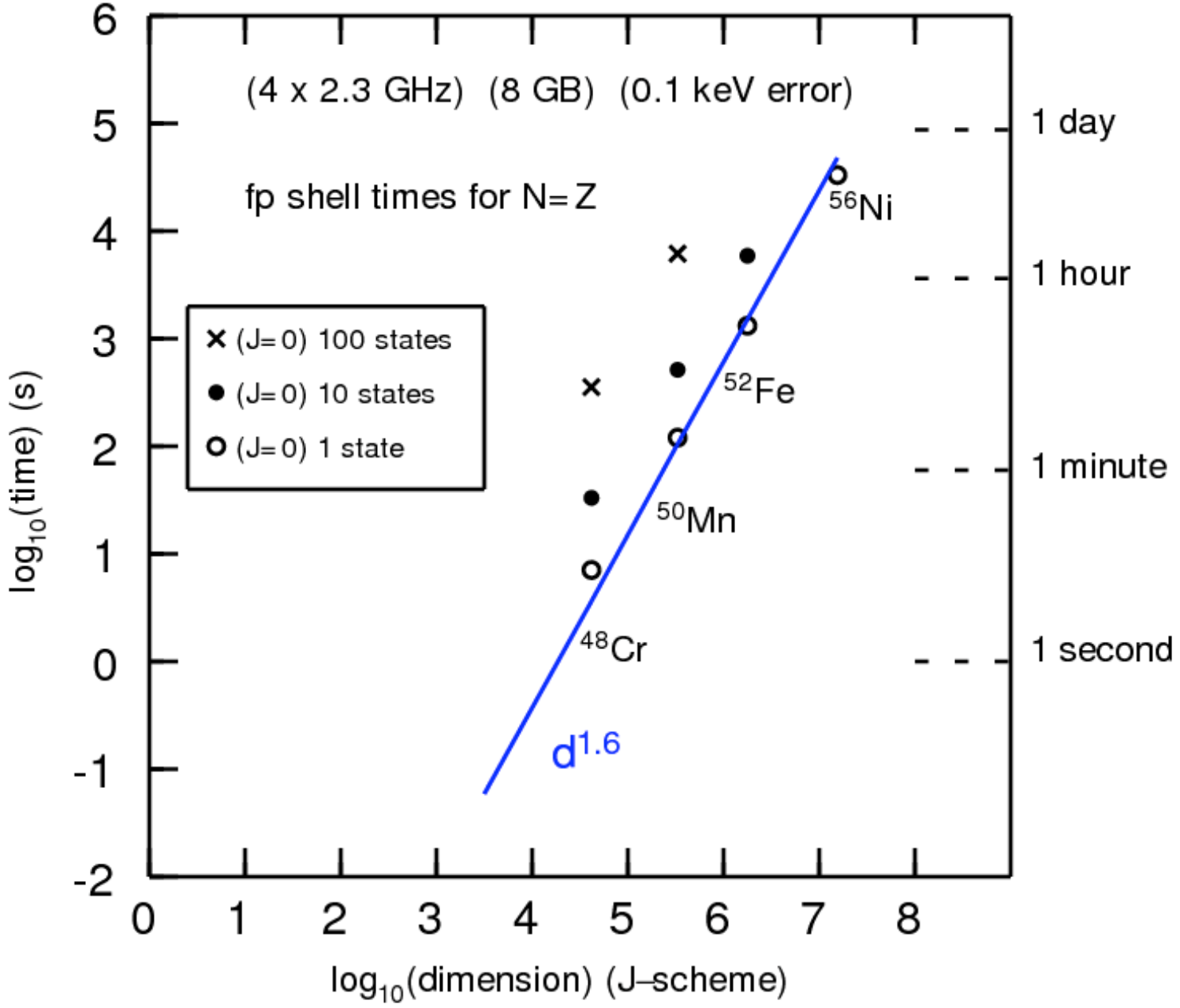
Extension of PCI:
Gao, Horoi PRC **79**, 014311 (2009), arXiv:0906.3756







Brown: Performance of the J-scheme code NuShellX



Shell-model CI codes and applications

Johnson, Krastev

Why "on-the-fly"?

Factorization of Hamiltonian (H) -> reduced memory
-> larger problem on same machine

10x faster than the old REDSTICK

Comparison of RAM requirements (2-body interactions only)

Does not include lanczos vector storage

Nuclide	Space	Basis dim	Half H store	BIGSTICK store
^{56}Fe	*pf*	501 M	290 Gb	0.72 Gb
^{7}Li	N_{max}=12	252 M	3600 Gb	96 Gb
^{7}Li	N_{max}=14	1200 M	23 Tb	624 Gb
^{12}C	N_{max}=6	32M	196 Gb	3.3 Gb
^{12}C	N_{max}=8	590M	5000 Gb	65 Gb
^{12}C	N_{max}=10	7800M	111 Tb	1.4 Tb
^{16}O	N_{max}=6	26 M	142 Gb	3.0 Gb
^{16}O	N_{max}=8	990 M	9700 Gb	130 Gb

Year 4 Deliverables

- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - Developed the charge-exchange QRPA code, and use it to study beta decay of nuclei in the r-process.
- **Bulgac, Stetcu, Magierski (UW), Roche (ORNL):**
  - Improve the generation of initial conditions for TD-SLDA, and study dilute fermion systems, and nuclear systems.
- **Horoi, Senkov, Central Michigan Unversity:**
  - Improve the scalability of the CI Moments code, and calculate the nuclear level densities for the heavier nuclei in the rp-process path. **It may require CS help.**
- **Brown, Michigan State University:**
  - Improve the scalability of the CI code NuShellX to hundreds of cores.
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of the new CI code REDSTICK up to 10,000 cores, and use it to investigate ^{12}C, ^{16}O ($N_{max}=8$) with 3-body interactions **(CS help needed).**

Future Plans: Year 5

- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - Develop the 2nd QRPA code and investigate the spreading widths of resonances.
- **Bulgac, Stetcu, Magierski (UW), Roche (ORNL):**
  - Use TD-SLDA ASDLA with consistent initial conditions to study nuclear spectral functions and nuclear reactions.
- **Horoi, Senkov, Central Michigan Unversity:**
  - Use CI techniques to investigate the double beta decay of ^{76}Ge, ^{82}Se, and ^{150}Nd.
- **Brown, Michigan State University:**
  - Use NuShellX to optimize the effective interaction for A=56-100 nuclei.
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of the new REDSTICK code up to 30,000 cores, and used to investigate ^{7}Li (N_{max}=12) with 3-body interactions.