

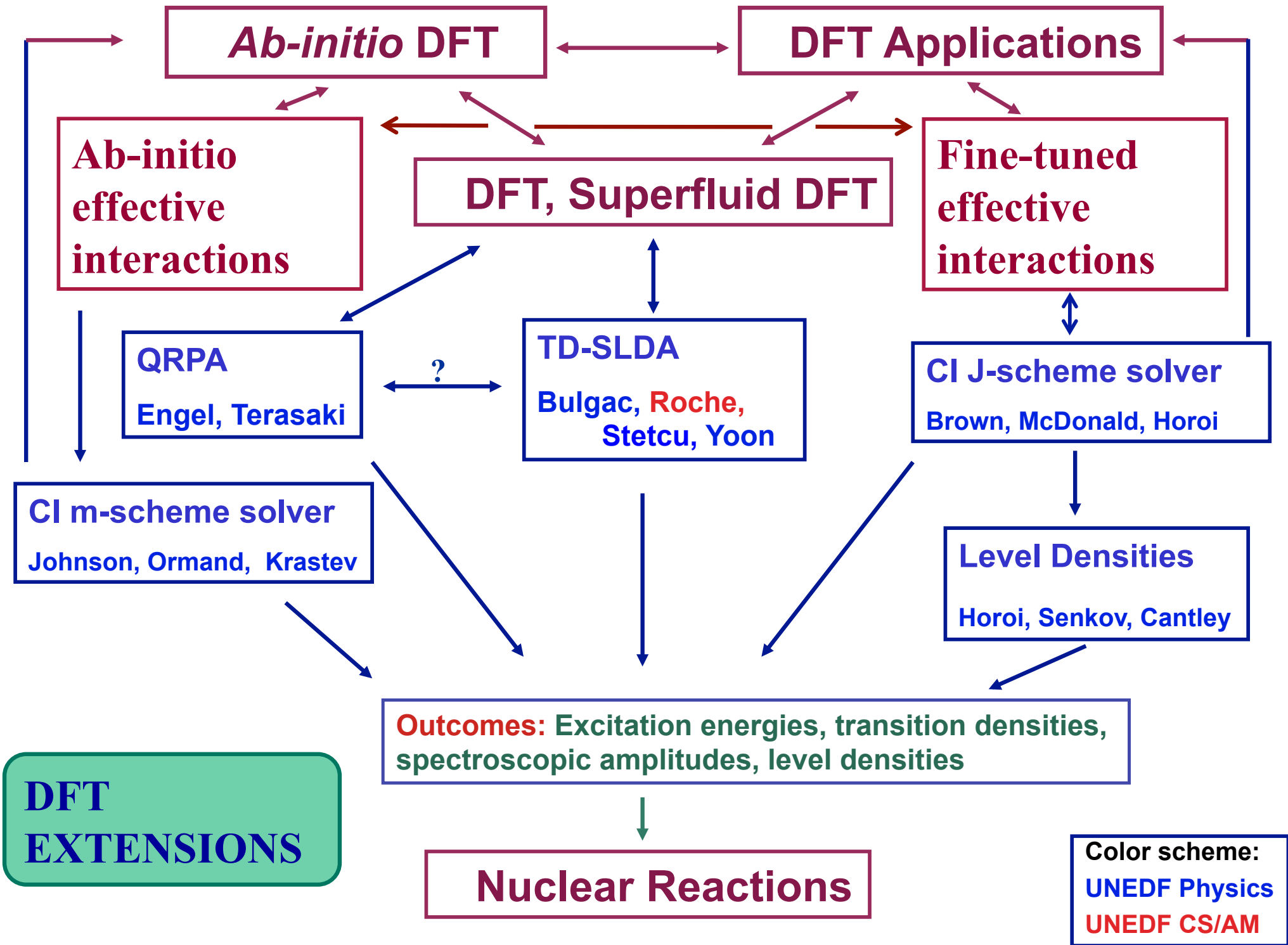
# Annual UNEDF Meeting 2010

**DFT Extensions:**

**Year-4 Deliverables**

**Year-5 Plans**

**Mihai Horoi - CMU**



# Year 4 Deliverables

## o 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.
  - ✓ Deformed QRPA code tested up to 10,000 cores; 2<sup>+</sup> systematics accomplished.
  - Charge-exchange code for  $\beta$  decay underway.

## o Bulgac, Stetcu, Magierski (UW), Roche (PNNL):

- Improve the generation of initial conditions for TD-SLDA, and study dilute fermion systems, and nuclear systems.
  - ✓ TD-SLDA study of dilute superfluid fermion system exhibiting vortices accomplished.
  - ✓ Few heavy nuclear systems investigated in the time dependent framework.

## o Horoi, Senkov, Central Michigan University:

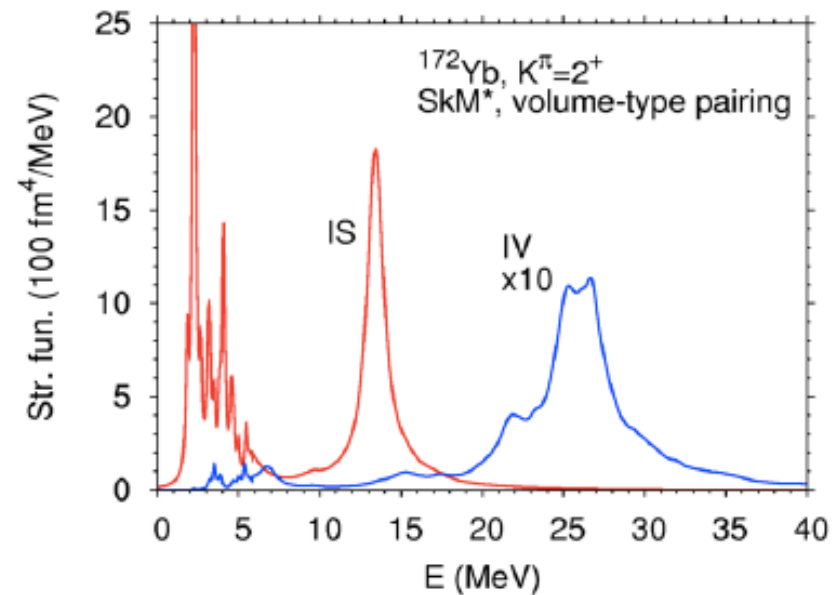
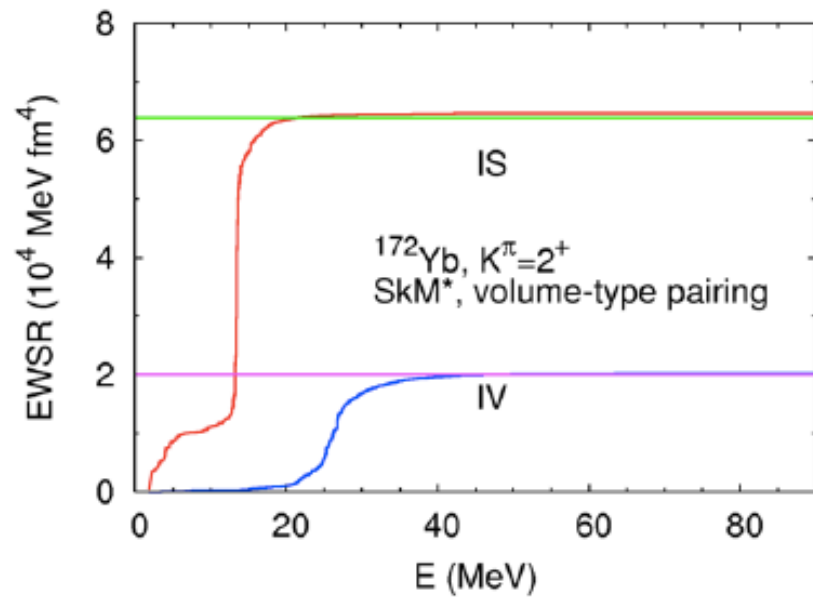
- Improve the scalability of the CI Moments code, and calculate the nuclear level densities for the heavier nuclei in the rp-process path. **It may require CS help.**
  - ✓ A new CI Moments code was developed using pn formalism, and its scalability was tested up to 4,000 cores.
  - ✓ Level densities and reaction rates for heavier nuclei in the rp-process path were calculated.
  - ✓ A new algorithm to determine the CI ground states energies was proposed and tested for <sup>64</sup>Ge and <sup>68</sup>Se.

# Year 4 Deliverables

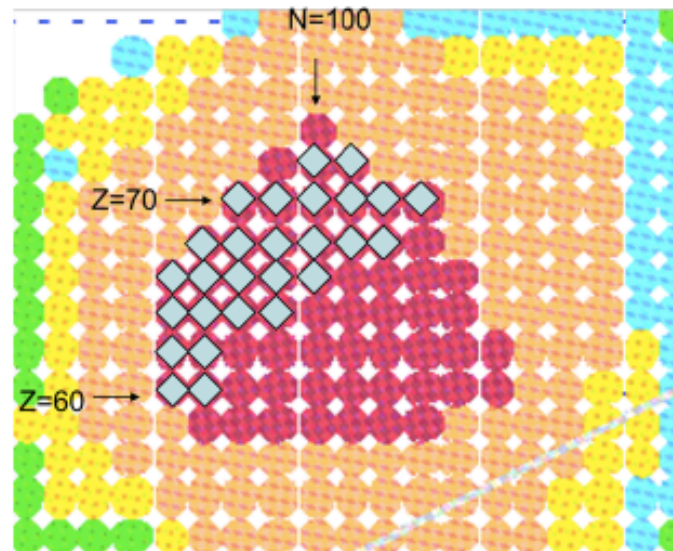
- o **Brown, Michigan State University:**
  - Improve the scalability of the CI code NuShellX to hundreds of cores.
    - ✓ NuShellX was successfully ported to the PGI compiler available at NERSC.
    - ✓ Code made available at the LCCI repository.
    - Study of scalability to hundred of processors with the PGI compiler underway.
- o **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of the new CI code BIGSTICK up to 10,000 cores, and use it to investigate  $^{12}\text{C}$ ,  $^{16}\text{O}$  ( $N_{\text{max}}=8$ ) with 3-body interactions (**CS help needed**).
    - ✓ matvec multiply for two-body code scales well up to 10,000 cores.
    - serial 3-body code in progress, will be finish by the end of year 4.
    - 3-body parallelization taking longer, will be finished in year 5.
- o **NEW - LCCI YEAR 4 Roadmap:**
  - ✓ LCCI codes and scripts delivered to UNEDF and are regularly updated.
  - ✓ Design/Prototype Data Base Managements System (DBMS) instituted.
  - ✓ Design/Prototype of unified wrapper for MFDn/BIGSTICK started.
  - ✓ NuShellX wrapper finalized.
  - ✓ Hands-on tutorial offered to UNEDF.

# Deformed QRPA Up and Running

## Electric-Quadrupole Strength in $^{172}\text{Yb}$

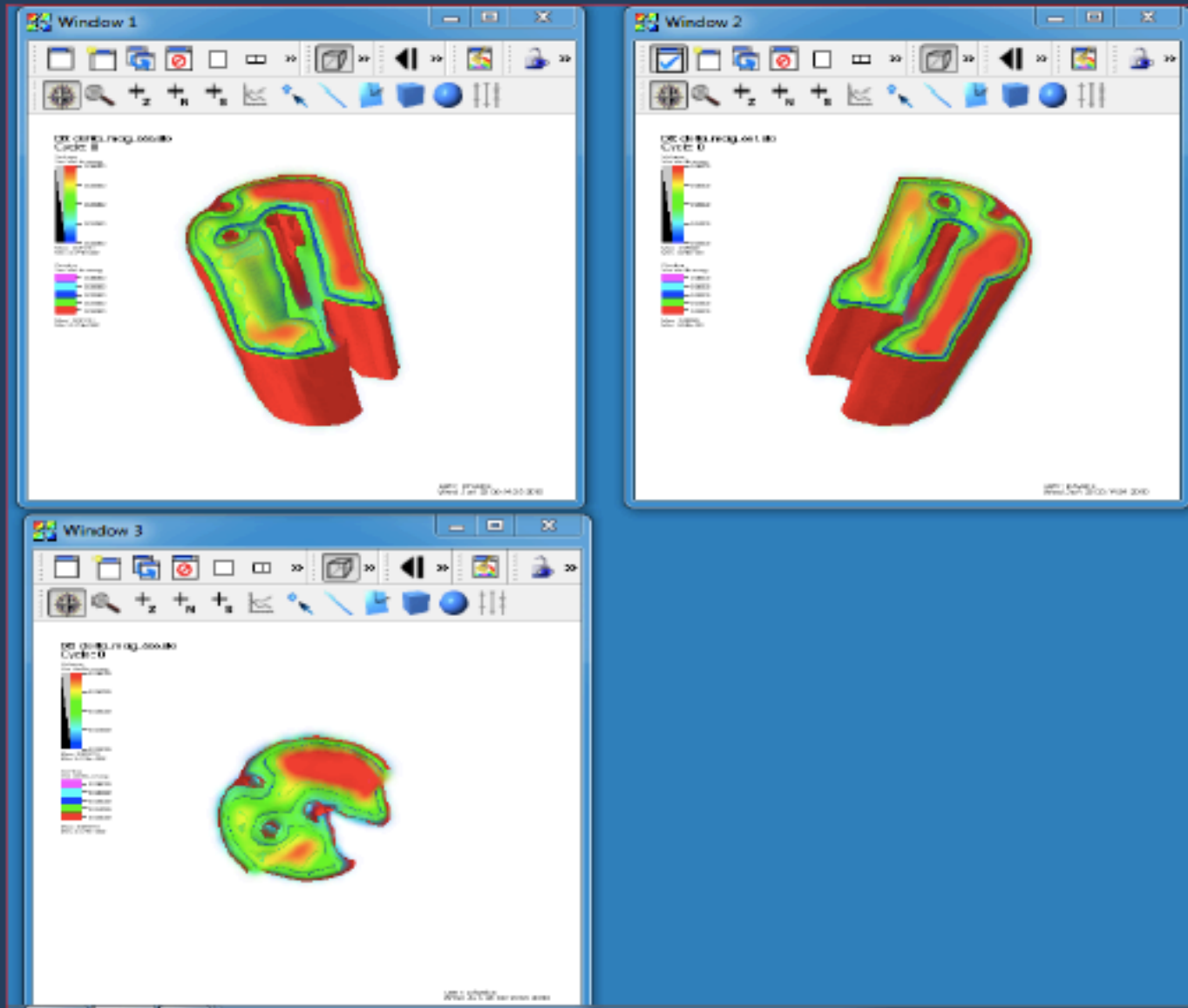


Study of Rare-Earths  
In Progress



- $\beta > 0.3$
- ◆ Lowest two  $2^+$  states measured

# Stirring of a unitary superfluid and generation of complex vortical motion by a rod and ball rotating in a cylindrical container



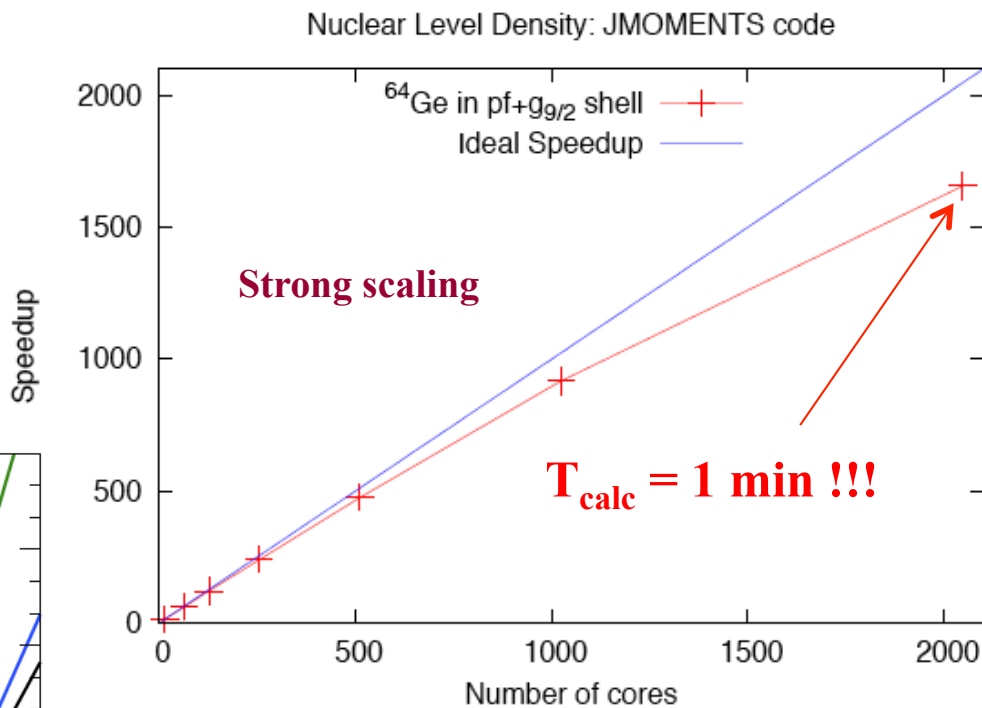
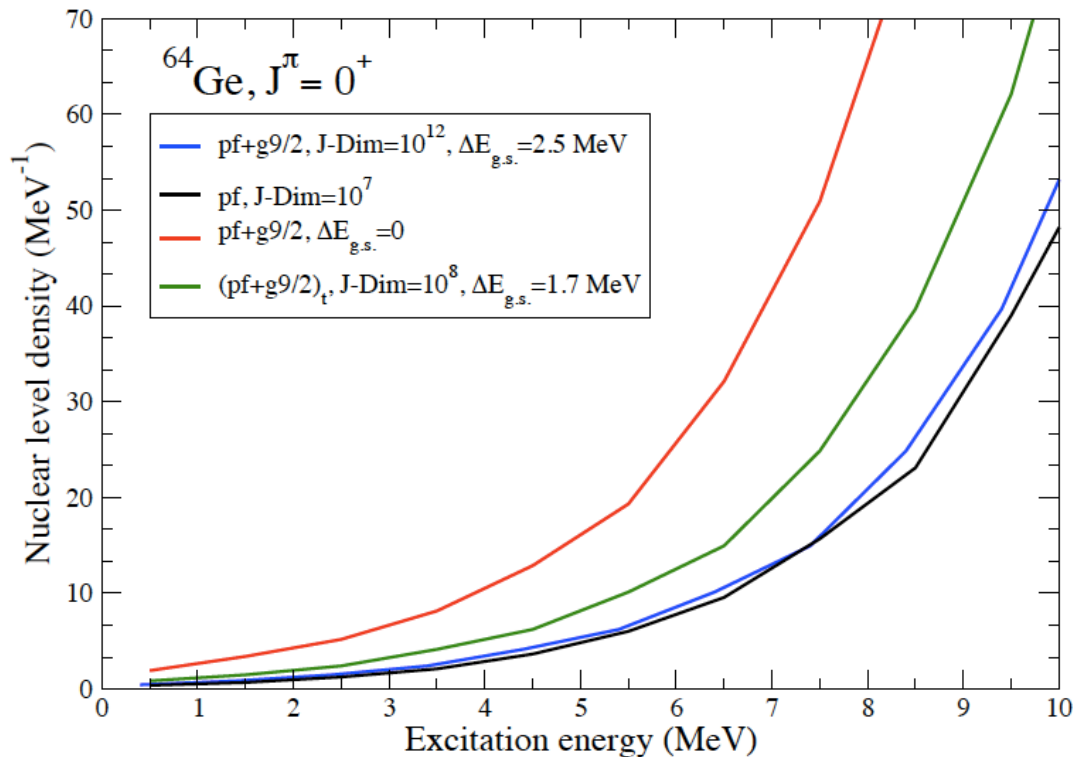
# Scalable JMOMENTS PN Code for Nuclear Level Density (NLD)

**Domain decomposition: many-body configurations**

**Algorithm: Dynamical Load Balancing**

**Machine: Franklin/NERSC**

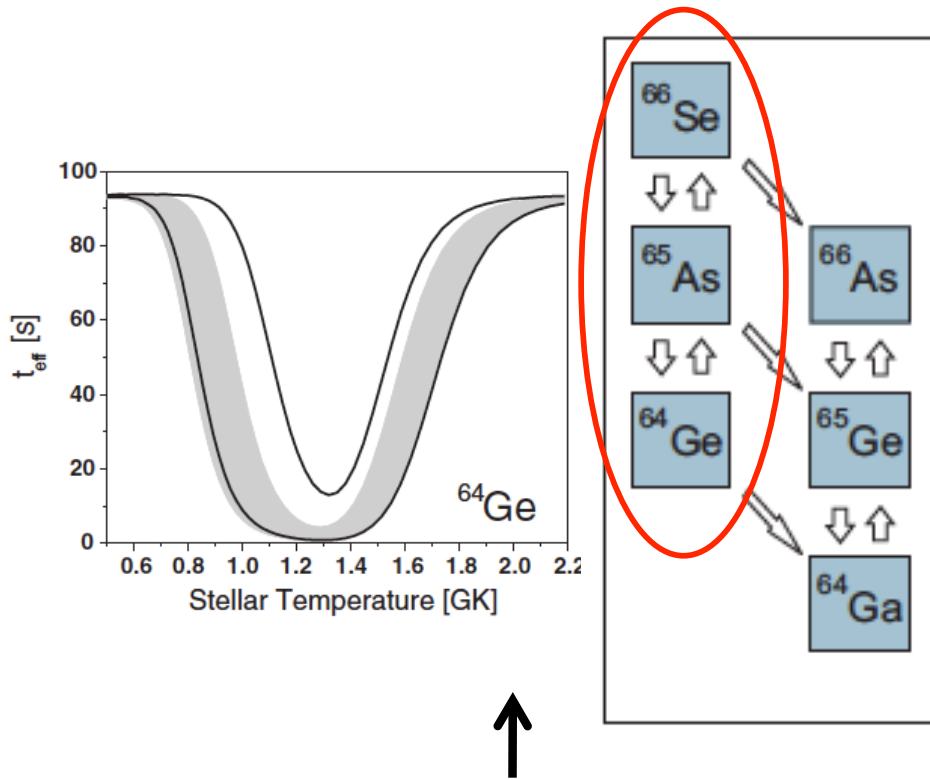
## New Algorithm for g.s. CI energy



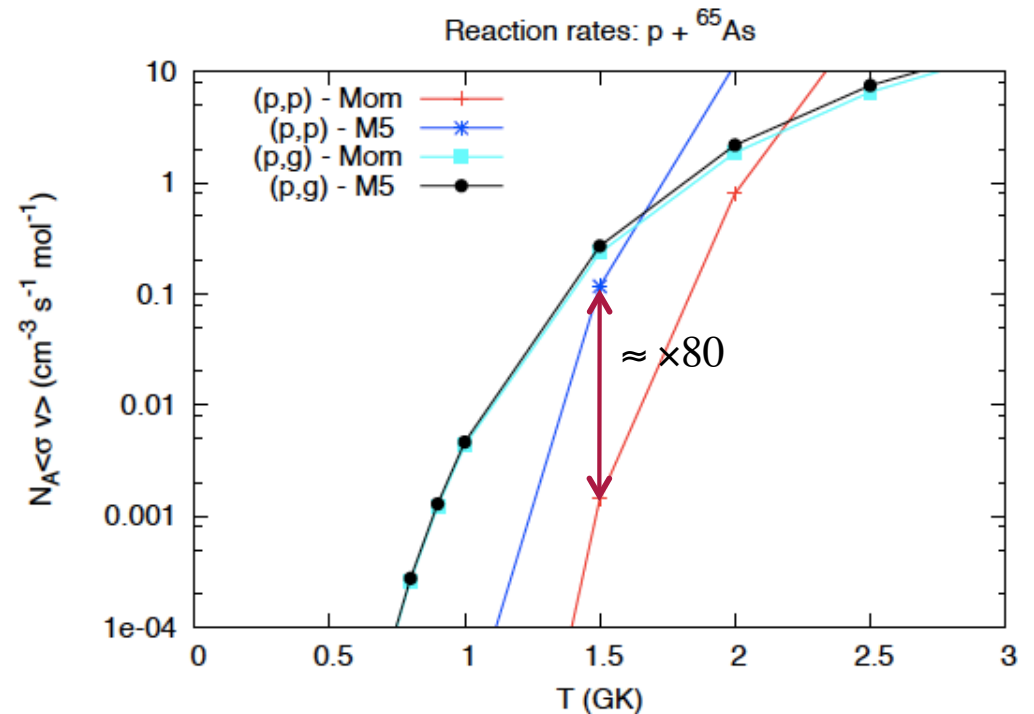
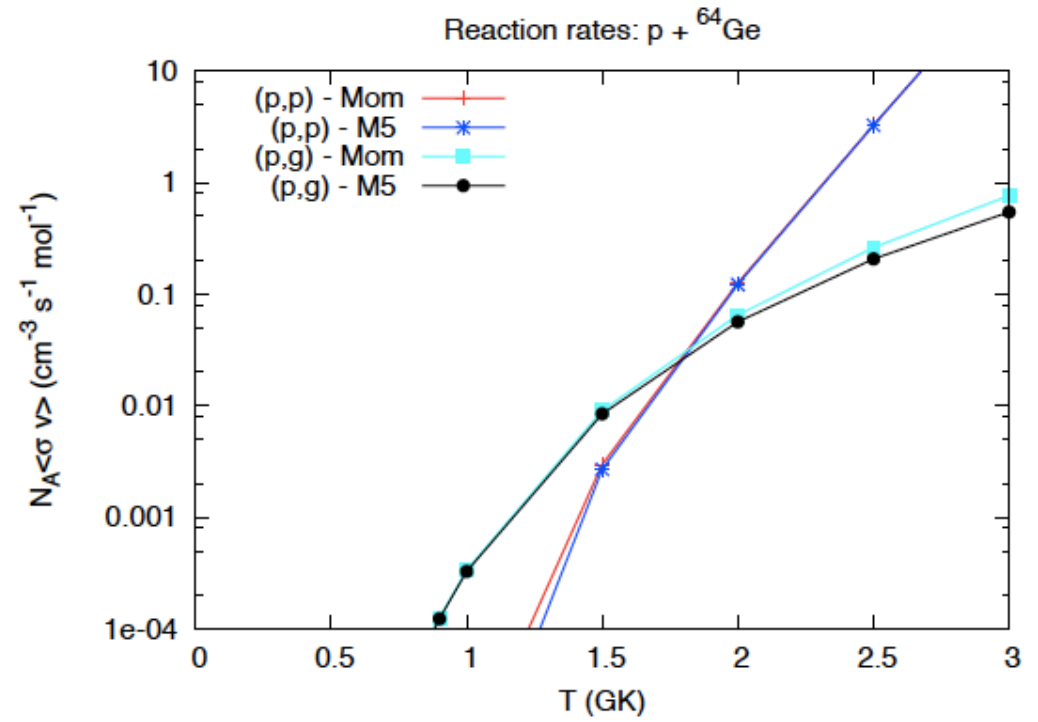
**m-scheme dimension ~ 10<sup>14</sup> !!!**

# First Calculation of Reaction Rates with CI NLD

Is  $^{64}\text{Ge}$  a “waiting-point” nucleus in the rp-process path?



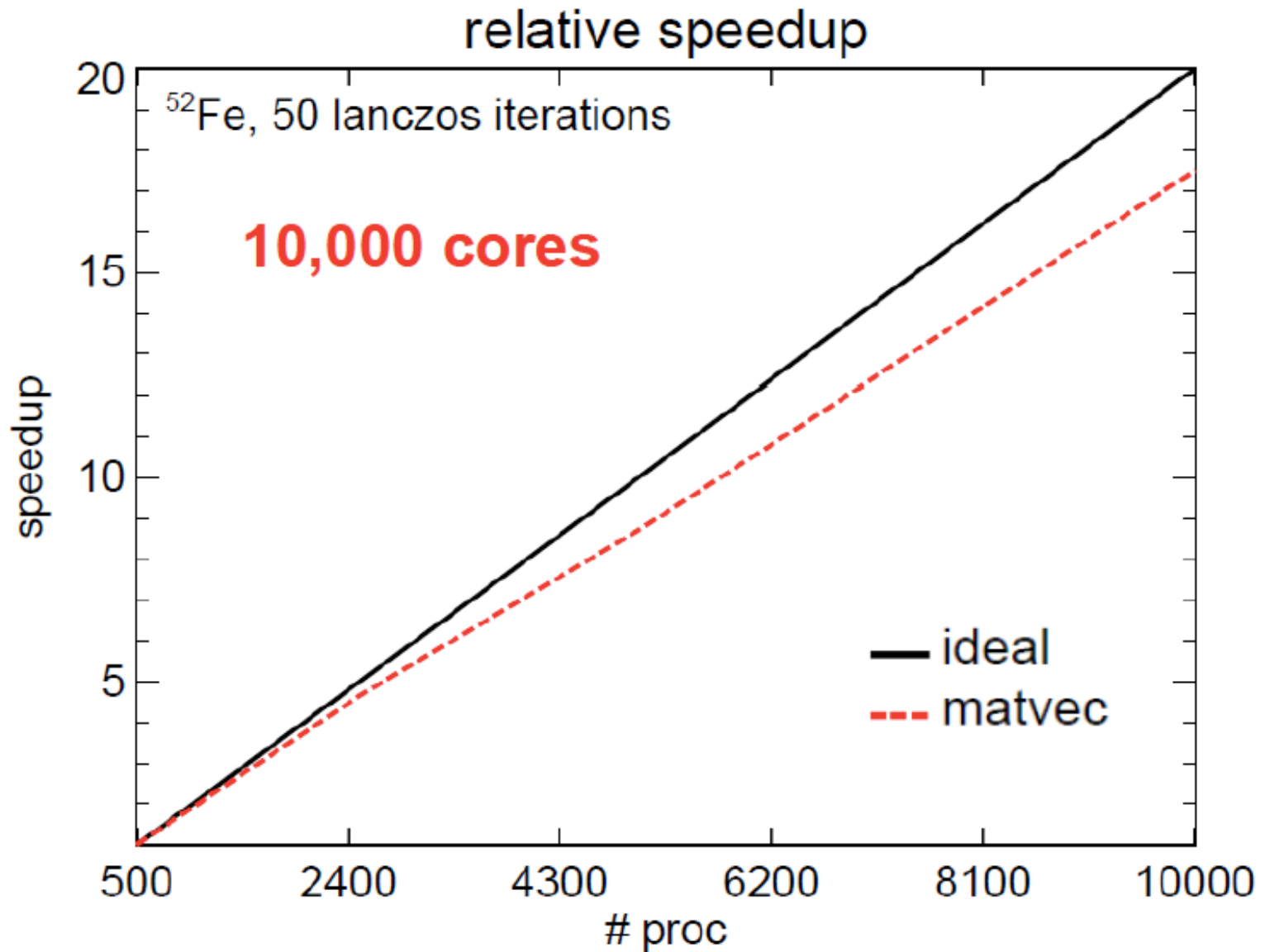
From P. Shury et al., PRC 75, 055801 (2007)





# BIGSTICK

(Relative) speedup of matrix-vector multiplication:



# Year 5 Plans

- **Engel, Terasaki, University of North Carolina at Chapel Hill:**
  - Complete calculation of  $\beta$  decay.
  - Develop DFT-consistent code beyond RPA.
- **Bulgac, Stetcu, Magierski (UW), Roche (PNNL):**
  - Improve the performance of the TD-SLDA code.
  - Test the small amplitude regime for light nuclei.
- **Horoi, Senkov, Central Michigan University:**
  - Develop and test the J-Moments NLD code that removes the center-of-mass spurious contributions.
  - Calculate more reaction rates in the rp-process path.
- **Brown, McDonald, Michigan State University:**
  - Understand the scalability barriers in NuShellX to enable the most effective use of GPUs and leadership-class machines.
- **Johnson, Krastev, San Diego State University, Ormand (LLNL):**
  - Improve the scalability of REDSTICK CI code up to 50,000 cores.
  - Use REDSTICK to investigate isospin breaking in pf shell.

# Year 5 Plans

- **Leadership Class CI Codes Effort:**
  - Complete a unified LCCI wrapper (ISU/MSU/SDSU)
  - Complete LCCI Data Base Management System (DBMS)
  - Final versions of UNEDF LCCI codes/scripts delivered to UNEDF