International Impact

Witold Nazarewicz (Tennessee)
DOE UNEDF Review, April 2008

International contributions
Exporting the knowledge and experience
Unique worldwide
Leveraging aspect
Unprecedented international effort
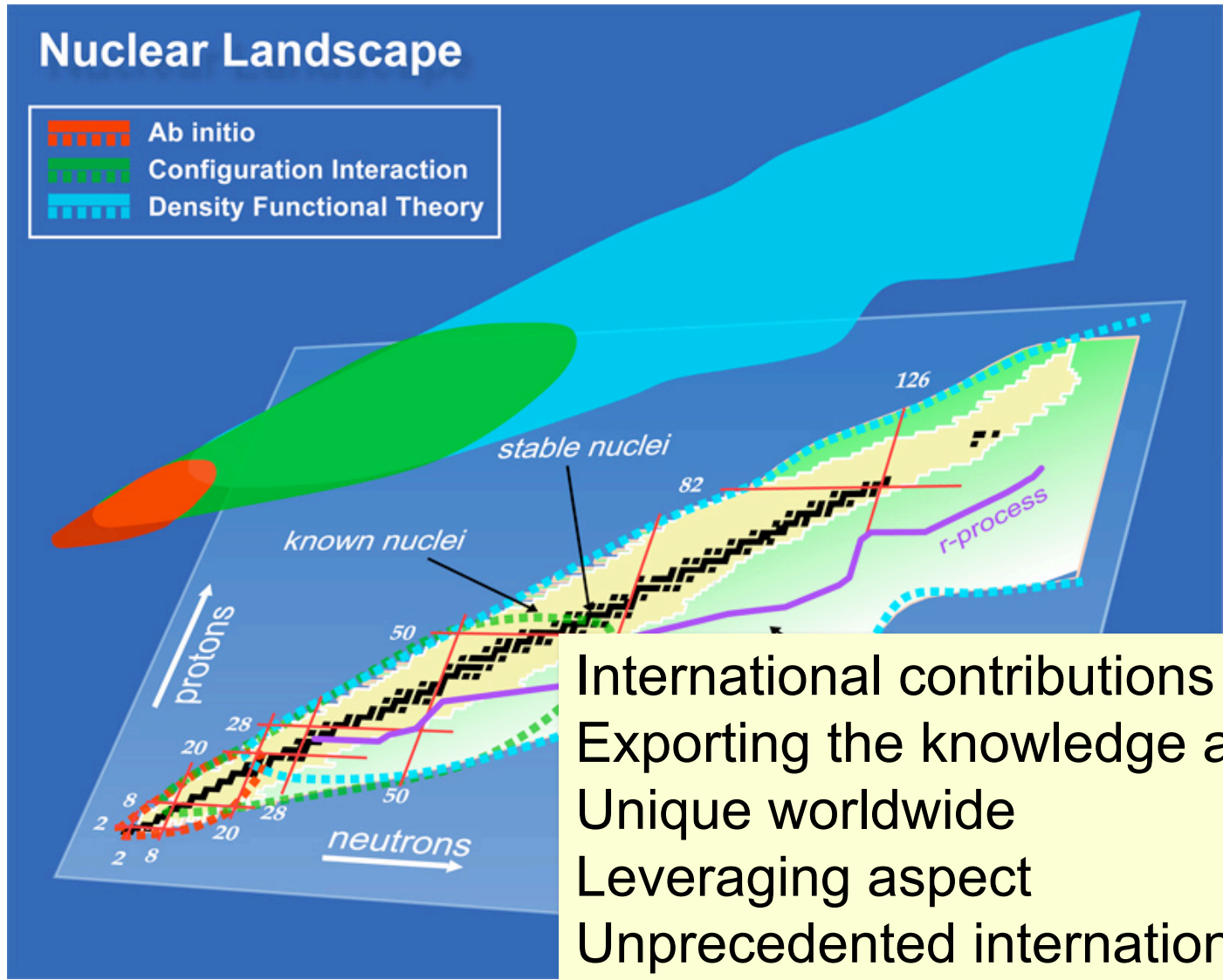
Participating Institutions and Investigators

Ames National Laboratory - M. Sosonkina
Argonne National Laboratory - M. Pervin, S. Pieper, R. Wiringa,
  E. (Rusty) Lusk, J. Moré, B. Norris
Lawrence Berkeley National Laboratory - E. Ng, P. Sternberg,
  C. Yang
Lawrence Livermore National Laboratory - J. Escher, P. Navratil,
  E. Ormand, S. Quaglioni, G. Stoitcheva, I. Thompson
Los Alamos National Laboratory - J. Carlson, M. Dupuis, T. Kawano,
  P. Möller
Oak Ridge National Laboratory - G. Arbanas, D. Dean, G. Fann,
  G. Hagen, K. Roche, W. Shelton
Central Michigan University - Z. Gao, M. Horoi
Iowa State University - P. Maris, J. Vary
Michigan State University - S. Bogner, B. Alex Brown, R. Sen'kov
University of North Carolina at Chapel Hill - J. Engel, J. Terasaki
Ohio State University - R. Furnstahl, L. Platter
San Diego State University - C. Johnson
Texas A&M Commerce - C. Bertulani
University of Tennessee - W. Nazarewicz, T. Papenbrock,
  N. Schunck, M. Stoitsov
University of Washington - G. Bertsch, A. Bulgac, S.-Y. Chang

M. Bender (Bordeaux, France)
J. Dobaczewski (Warsaw, Poland; Jvyäskylä, Finland)
T. Duguet (Saclay, France),
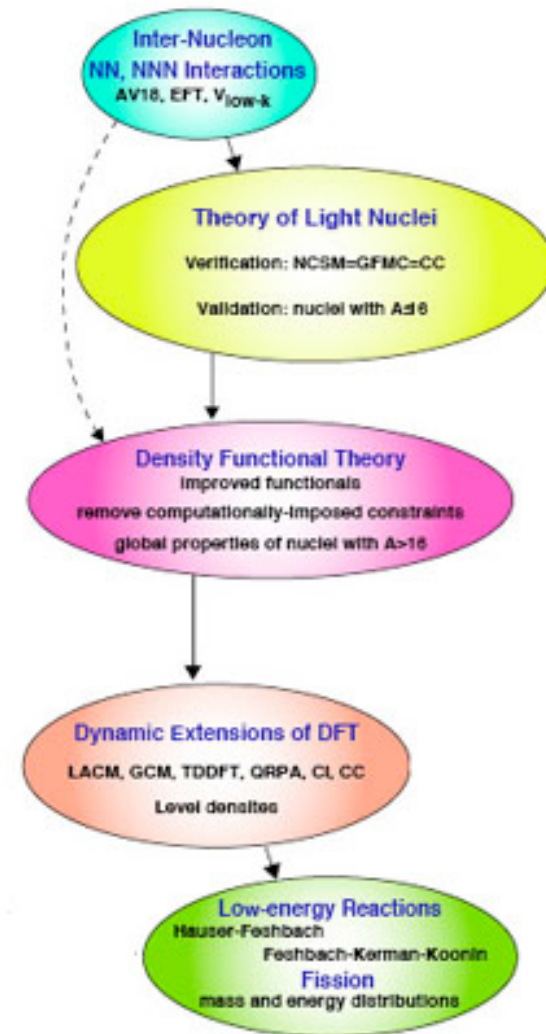H. Goutte (Bruyères-le Châtel, France)
P.-H. Heenen (Brussels, Belgium)
P. Magierski (Warsaw, Poland)
T. Nakatsukasa (RIKEN, Japan)
A. Schwenk (TRIUMF, Canada)

Universal Nuclear Energy Density Functional

Inter-Nucleon
NN, NNN Interactions
AV16, EFT, V_{low-k}

Theory of Light Nuclei
Verification: NCSM=GFMC=CC
Validation: nuclei with A≤16

Density Functional Theory
Improved functionals
remove computationally-imposed constraints
global properties of nuclei with A>16

Dynamic Extensions of DFT
LACM, GCM, TDDFT, QRPA, CI, CC
Level densities

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

Color denotes:

- Physics
- Computer Science & Applied Mathematics
- Foreign Collaborators

Europe

Warsaw-Jyväskylä

Paris-Bordeaux-Bruyeres-Lyon-Brussels

- Joint code developments
- Defining optimization strategy
- New Joint Research Activity on Nuclear Structure Theory (under EURONS-2); Helsinki Town Meeting September 17-19
- ARTHENSA proposal to the ESF

Japan

- Joint activities (via JUSTIPEN)
- Workshop July 2008 in Hokkaido
- Helping to build the case for petascale nuclear structure initiative around RIKEN

The 2nd LACM-EFES-JUSTIPEN Workshop

Joint Institute for Heavy Ion Research, Oak Ridge, Tennessee, USA
Oak Ridge National Laboratory
January 23-25, 2008

Time	Speaker	Title
8:30	D. Dean, G. Young, and T. Otsuka	Opening
8:45-10:15	G. Hagen	Coupled-cluster Theory for Nuclei
	S. Fujii	Structure of sd- and pf-shell Nuclei with Microscopic Effective Interactions
	J. Vary	Full Configuration Interaction Studies of Light Nuclei – Opportunities and Challenges (ppt version)
	Y. Utsuno	Large-scale Shell Model Calculations for Exotic Nuclei
10:30-11:30	*Ceremony (JIHIR / JUSTIPEN) program to be announced*	
11:30	B. Shelton	Implementing Density Functional Theory based Electronic Structure Code on Advanced Computing Architectures (ppt version)
	D. Kothe	The National Center for Computational Sciences at Oak Ridge: overview and roadmap
12:30	*LUNCH*	
1:30	J. More	A Short Guide to Optimization Technology on High-Performance Architectures
	M. Stoitsov, N. Schunck	Large-scale mass table calculations with DFT (ppt version)
		Spectroscopy of Odd-Mass Nuclei (ppt version)
	Y. Kanada-En'yo	Cluster Model Calculations
2:45	*COFFEE*	
3:00	Tour of Jaguar	
4:00	A. Ono	Time-Dependent AMD Calculations for Reactions
	J. Rotureau	Density Matrix Renormalization Group Approach for Many-Body Open Quantum Systems
	T. Mezzacappa	When micro and macro worlds meet: modeling core collapse supernovae
5:00	Discussion on Supercomputing in low-energy nuclear physics (Leaders: D. Dean and T. Nakatsukasa)	

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DFT-UNEDF Workshop

Determination of the Nuclear Energy functional: Optimization Strategy, Essential Experimental Data and Chi-Squared Metrics

Joint Institute for Heavy Ion Research, ORNL,
Oak Ridge, TN-37831, USA
January 22, 2008

41 participants

Talks

Name	Title of Contribution	File
A. Brown	Strategies for Extracting Optimal Effective Hamiltonians for CI and Skyrme EDF Applications	Brown.ppt
J. Dobaczewski	Spectroscopic-Quality Energy Density Functional and How to Get There	Dobaczewski.ppt

Choice of Experimental Observables

Name	Title of Contribution	File
A. Afanasjevs	Terminating States: Can They Be Used to Constrain DFT ?	Afanasjevs.pdf
G. Colo	Constraints from Collective States	Colo.ppt
P. Kluepfel	Best Mean-Field Nuclei for Fits	Kluepfel_1.pdf
P. Kluepfel	Fitting Strategies	Kluepfel_2.pdf
H. Sagawa	Constraints to Universal Energy Density Functionals by Giant Resonances	Sagawa.ppt
N. Schunck	Large Deformations in DFT Fits	Schunck_1.ppt
N. Schunck	Quasi-particle Spectra in DFT Fits	Schunck_2.ppt
J. Terasaki	QRPA Calculation in Fitting Process of Functional	Terasaki.ppt
J. Vary	Ab-initio calculations with an external field - initial results	Vary.ppt

Minimization and Algorithms

Name	Title of Contribution	File
K. Bennaceur	Stability Criteria for Skyrme Energy Functionals	Bennaceur.pdf
J. Moré (1)	Validation of Models	More_1.pdf
J. Moré (2)	Parameter Estimation in Nuclear Fission	More_2.pdf
T. Lesinski	Minimization Algorithms for Local and Global Minima Search	Lesinski.pdf

http://orph02.phy.ornl.gov/workshops/lacm08/unedf.html

Summary

- International contributions
- Exporting the knowledge
- Exporting the SciDAC experience
- Physics/CS/AM coupling unique worldwide
- Leveraging aspect: creating new initiatives abroad
- Unprecedented international effort