Scattering Function S(a,b) Covariance

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Direct Capture Reactions

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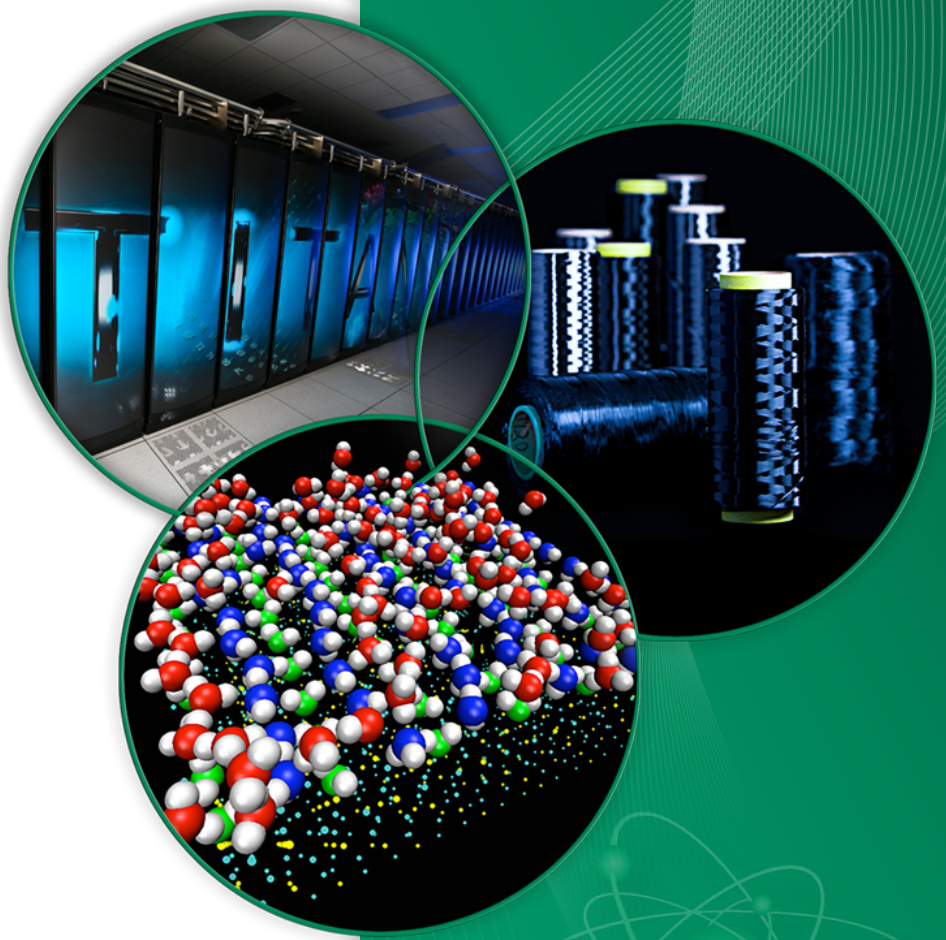

Nuclear Data Week; USNDP Reaction Modeling
November 18-22, 2013, BNL, NY

Overview

- Goal: Develop methods for generating covariance data of S(a,b)
  - In anticipation of the RPI data for H_20 and $Si0_2$ (Si) from the SNS
- General approach:
  1. Define model T as a function of some parameters P
  2. Fit model T to data to obtain covariance matrix M of parameters P
  3. Construct covariance of S(a,b) from M as C = S M S
     - Where $S = \partial T(P) / \partial P$ is the sensitivity matrix of model T
- Various models T being considered:
  - Addressing various levels of physical models
    - Various approximations: from DFT to MD to free gas,
    - Some assumptions revisited (e.g. form of the scattering w.f.)
  - *Ab intio* models more computationally intensive
- MADNESS Computational framework (R&D 100, SciDAC)
  - May provide novel computational approaches and insights

General consideration

- The form of the scattering function assumed
  - Plane wave + scattered wave
  - Can we estimate the magnitude of ensuing error? (assumed to be small)
- The low-energy (< 5 eV) neutron-nucleus scattering determined by the scattering length
- First-order Born approximation
  - Does not require a delta-function interaction;
    - Woods-Saxon is more realistic
    - But delta-function is likely a good approximation since size(nuclei) << size(atoms)
- This leads to expressions for S(a,b) in terms of pair-wise correlation functions
  - Delineates neutron-scattering from material properties PCF
  - →PCF could be computed by e.g. MD or DFT
- What is an efficient path to S(a,b) covariance?

1. Molecular Dynamics (MD)

- MD Method:
  - assumes a parameterized interaction potential (e.g. Lennard-Jones)
  - Uses Newton's equation to evolve the many-body system
  - Then computes PCFs to get S(a,b) and structure factors
  - Faster but less accurate than more ab initio methods like DFT
  - Interaction parameters fitted to (usually) structure factors (SF)
  - The SF is the 0-th moment of S(q,w)
  - But parameter uncertainty or covariance is generally not provided
- Several established MD codes available
  - GROMACS
  - NAMD
  - http://en.wikipedia.org/wiki/List_of_software_for_molecular_mechanics_modeling

2. Density Functional Theory

- Codes:
  - BigDFT, MADNESS (more later)
  - http://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid_state_physics_software
- Water is still not fully understood
  - Discrepancies between data an theory persist
    - structure factor, pairwise correlation function
  - Several recent Ph.D. thesis on water (active field)
- ~1,000's of atoms/molecules
- More accurate than MD
- DFT computations are used to fit MD interaction parameters
- A candidate framework for S(a,b) covariances

3. Horace platform

- One of the two preferred methods for data reduction and analysis
  - at the SNS Sequoiah
  - double diff. (angle, energy) cross section is reduced to $S(\mathbf{q},\omega)$
  - Built-in function for parameter fitting to reduced data $S(\mathbf{q},\omega)$
    - Returns model parameters, their uncertainties, and the correlation matrix
    - One can compute the model covariance matrix of the $S(\mathbf{q},\omega)$

- An established platform
  - Works with MATLAB out of the box
  - Used in multitude of advanced papers
  - Downloadable from http://horace.isis.rl.ac.uk

MADNESS
An Introduction

Multiresolution
Adaptive
Numerical
Scientific
Simulation

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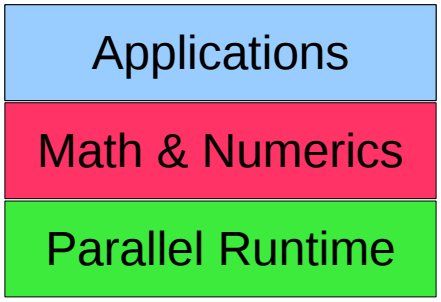
What is MADNESS?

- A general purpose numerical environment for reliable and fast scientific simulation
  - Chemistry, nuclear physics, atomic physics, material science, nanoscience, fluidics ...

- A general purpose parallel programming environment designed for the peta/exa-scales
  - Standard C++ with concepts from Cilk, Charm++, Intel TBB, HPCS languages
  - Compatible by design with existing applications
  - Runs on the *world's* largest computers

What is MADNESS?

- MADNESS is a framework
  - Like NWChem, PETSc, ...



- Frameworks
  - Increase productivity; hide complexity
  - Interface disciplines; capture knowledge
  - Open HPC to a wider community
  - Long-lived, communal projects with broad impact
  - 2011 R&D 100

Why MADNESS?

- MADNESS addresses many of the sources of complexity that constrain our HPC ambitions
  - Science, physics, theory, ...
    - Constantly evolving but can take years to implement
  - Scalable algorithms and math
    - Need rapid deployment of the latest and greatest
  - Software
    - Crude parallel programming tools with explicit expression and management of concurrency and data
  - Hardware
    - Millions of cores with deep memory hierarchy

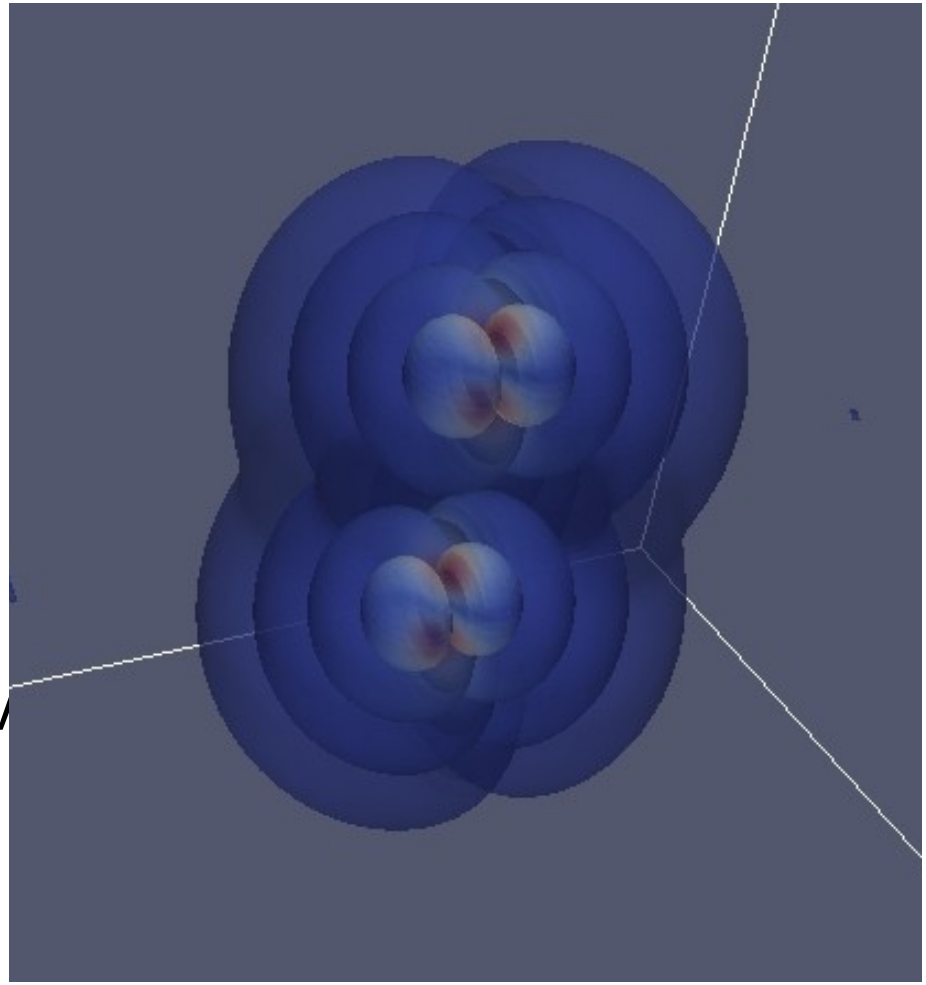
Why MADNESS?

- Reduces S/W complexity
  - MATLAB-like level of composition of scientific problems with guaranteed speed and precision
  - Programmer not responsible for managing dependencies, scheduling, or placement
- Reduces numerical complexity
  - Solution of integral not differential equations
  - Framework makes latest techniques in applied math and physics available to wide audience

Nuclear physics

J. Pei, G.I. Fann,
W. Nazarewicz
UT/ORNL

- DOE UNDEF/NUCLEI
- Nuclei & neutron matter
- Cold Fermions
- Hartree-Fock-Bogliobulov
- Spinors
- Gamow states



Imaginary part of the seventh eigen function
two-well Wood-Saxon potential

An alternative view of fitting methods

- Wavelets in the context of image processing give an alternative vista for fitting methods
  - It places Bayes method into a broader context
    - Unrealistically small uncertainties
  - Relative to the Minimax alternative
  - The optimal fitting is likely in between the two

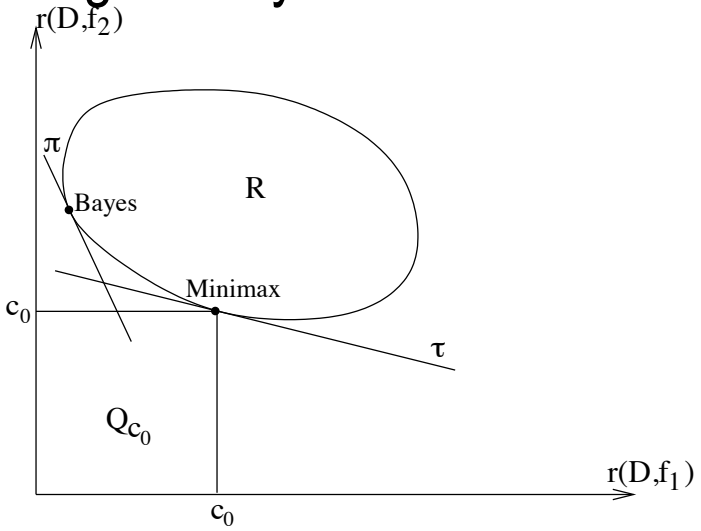


Figure 11.3: At the Bayes point, a hyperplane defined by the prior π is tangent to the risk set R. The least favorable prior τ defines a hyperplane that is tangential to R at the minimax point.

Conclusions and Outlook

- Various approaches for computing S(a,b) outlined
- Prospect of using MADNESS wavelet framework explored

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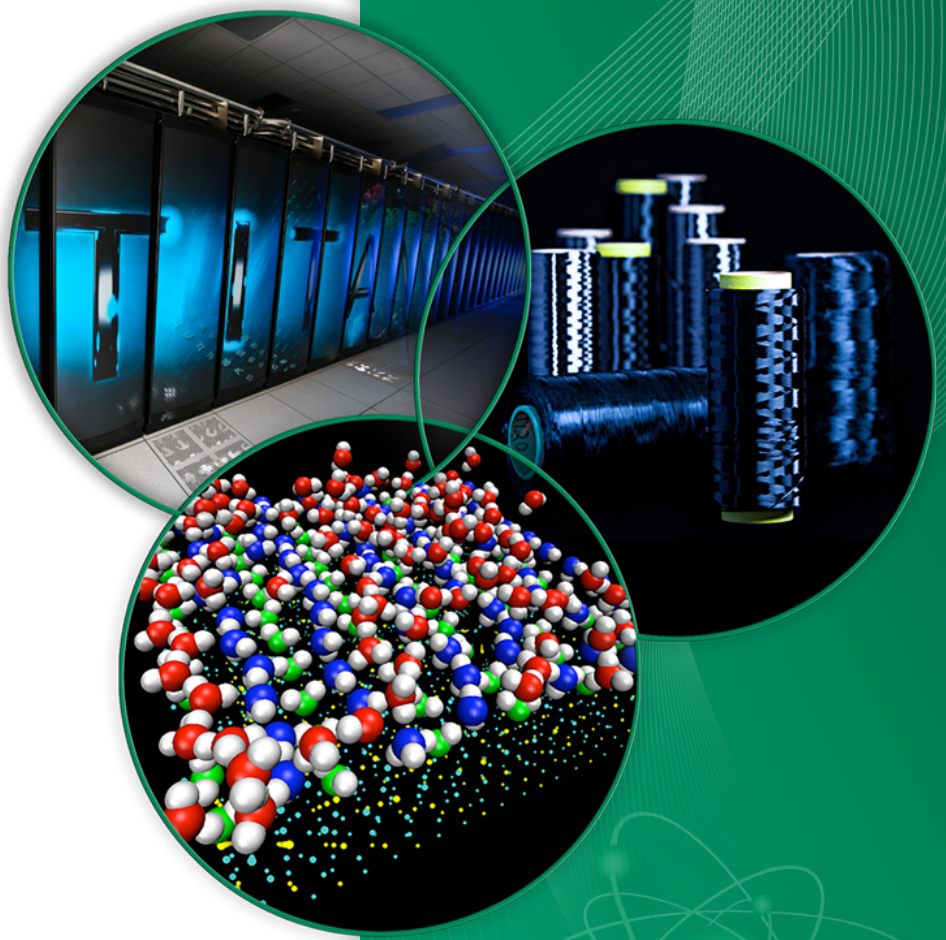

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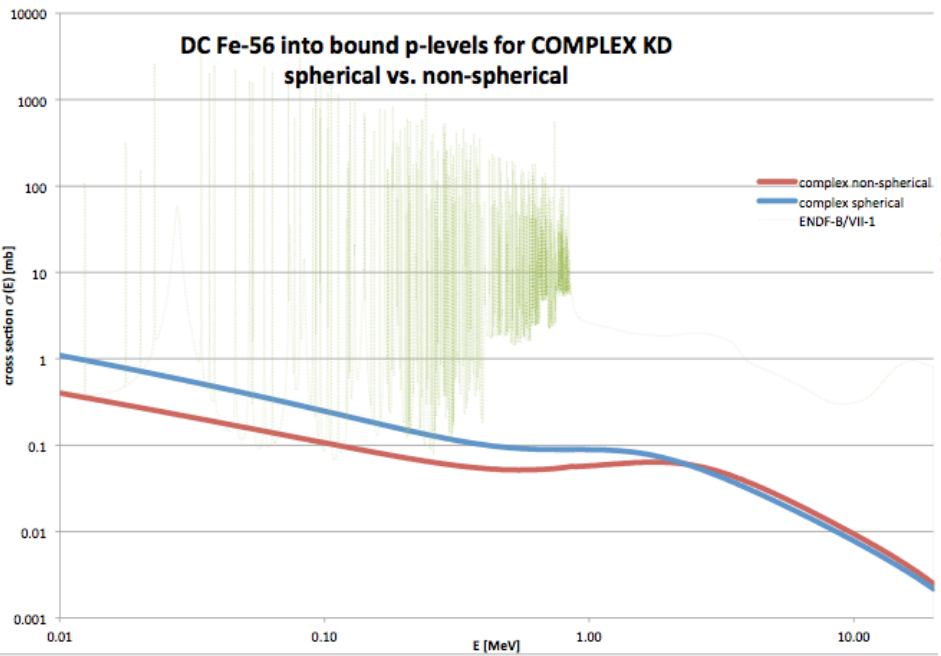
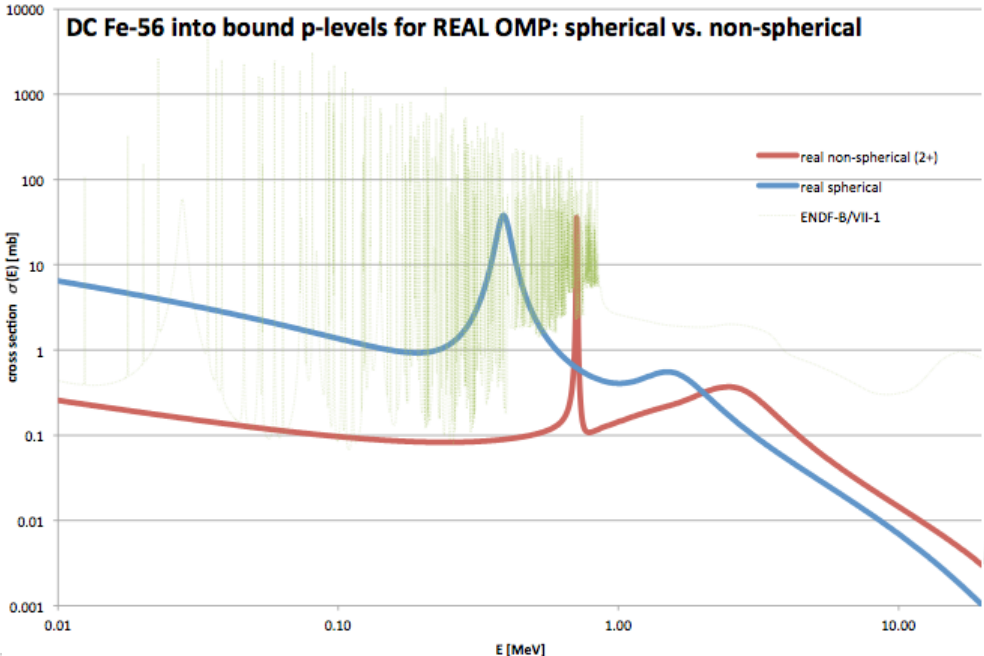
Coupled channels capture

- Neutron-nucleus scatterings require coupled- channels calculations.
  - Rotation models for all known band, even beyond
  - Vibrational models for 1- or 2-phonon excitations
- For consistency, should include these couplings also in the final neutron bound states.





Gamow Shell Model CC Neutron Capture

- Motivated by the need for neutron capture c.s. on unstable Sn-130
  - TORUS in support of HRIBF experiment Sn-130(d,p) (Kozub et al.)
- Collaboration with Nicolas Michel (MSU) et al.
- ORNL Small Seed Money proposal (synergistic w/ TORUS):

The amplitude for the capture of an incoming nucleon of energy E_n in a channel labeled by a composite index "c" relative to an (A-1) target nucleus is expressed via the T-matrix to the first-order in the electro-magnetic operator H_γ [1]:

$$\frac{d\sigma_{fc}}{dE_\gamma d\Omega_\gamma} = \frac{1}{\phi_{\rm inc}} \frac{2\pi}{\hbar} \frac{E_\gamma^2}{(\hbar c)^3} |T_{fc}|^2 \delta(E - E_f)$$

$$T_{fc} = \langle \Psi_f^{(A)} | H_\gamma | \Phi_c \rangle$$

"GSM-CC" incoming channel wave functions $|\Phi_c\rangle$

GSM final bound levels of the (A) nucleus $|\Psi^{(A)}\rangle$

Jaganathen Y, Michel N, Płoszajczak M 2013 arXiv:1210.1927v1 [nucl-th]

Conclusions and Outlook

- New coupled-channel approaches to capture
  - Fresco: coupling to 2+ states in incoming and outgoing channels
    - Self-consistent approach to capture on deformed nuclei
    - Apply to the chain of even Ca isotopes
  - Gamow-Shell Model Coupled Channels
    - Model more complex configurations in the capture process 2p-1h, …