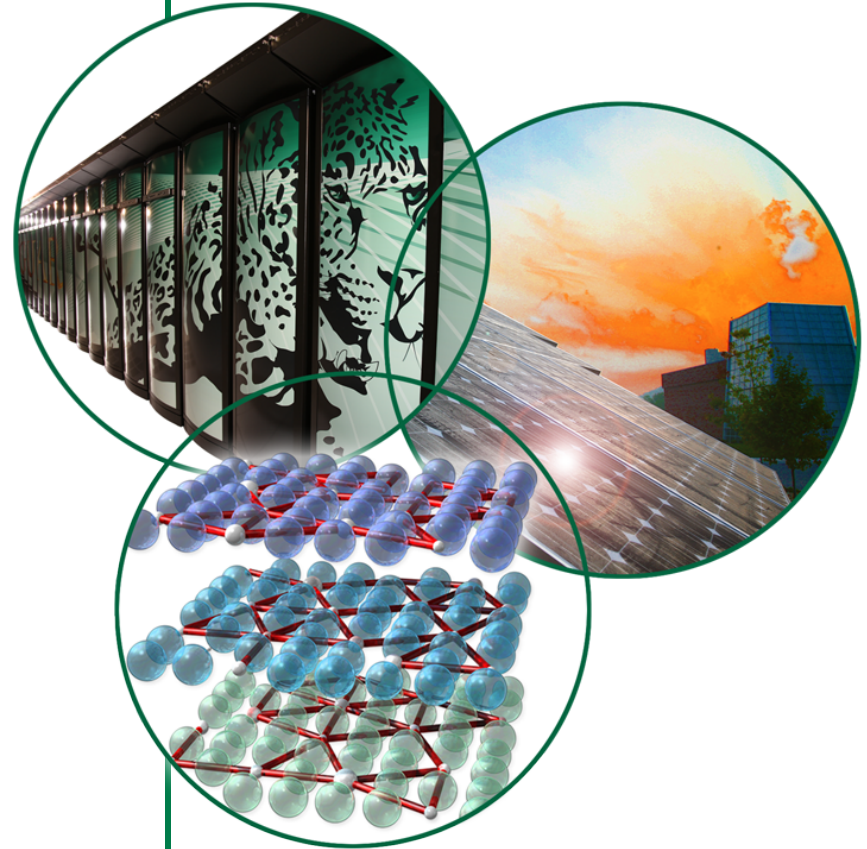


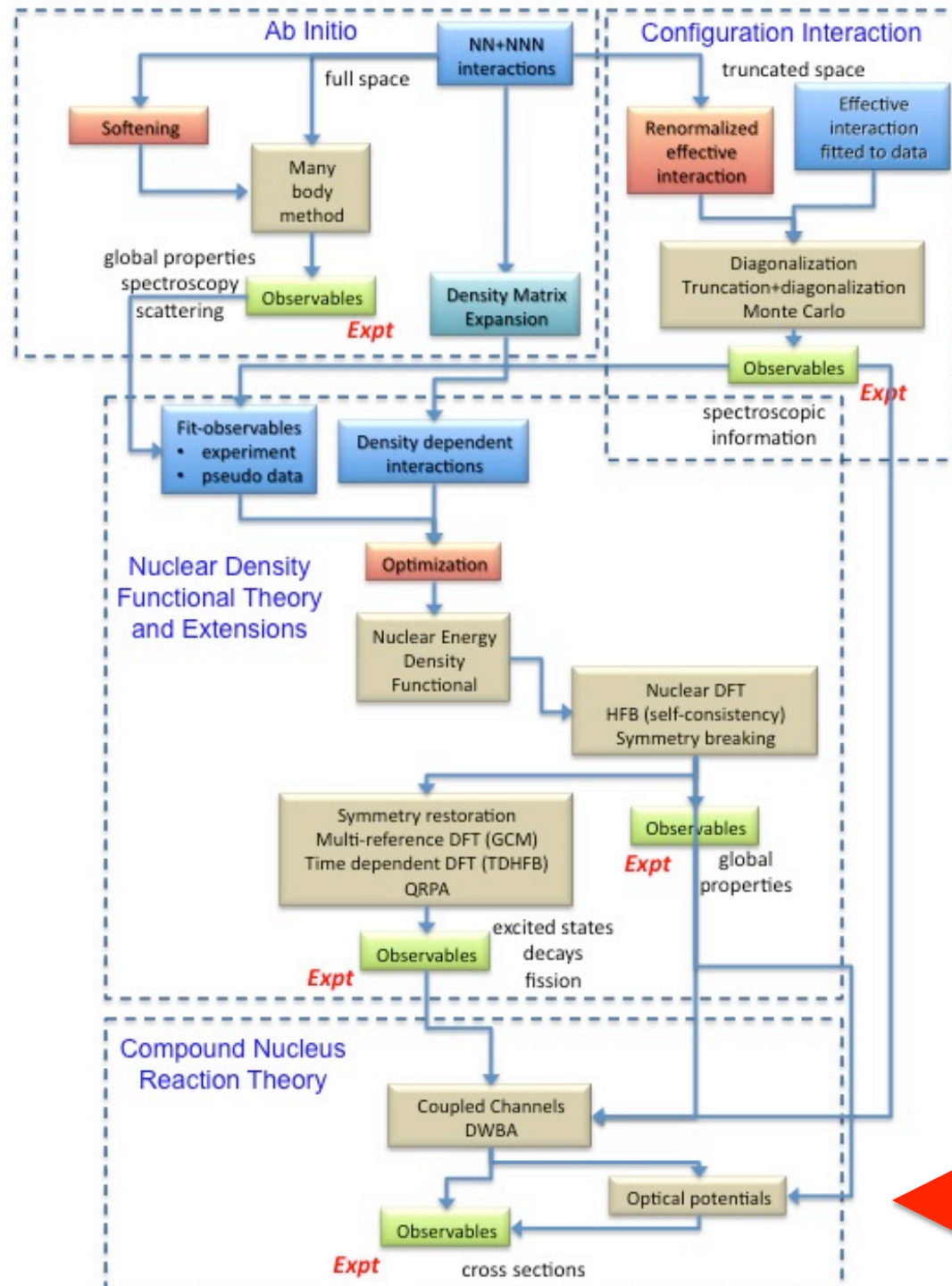
Statistical Theory of Nuclear Reactions

UNEDF SciDAC Annual Meeting

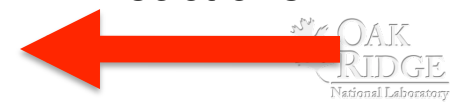
MSU, June 21-24, 2010

Goran Arbanas (ORNL)
Kenny Roche (PNNL)
Arthur Kerman (MIT/UT)
Carlos Bertulani (TAMU)
David Dean (ORNL)





HPC numerical simulation of formal theories of statistical nuclear reactions



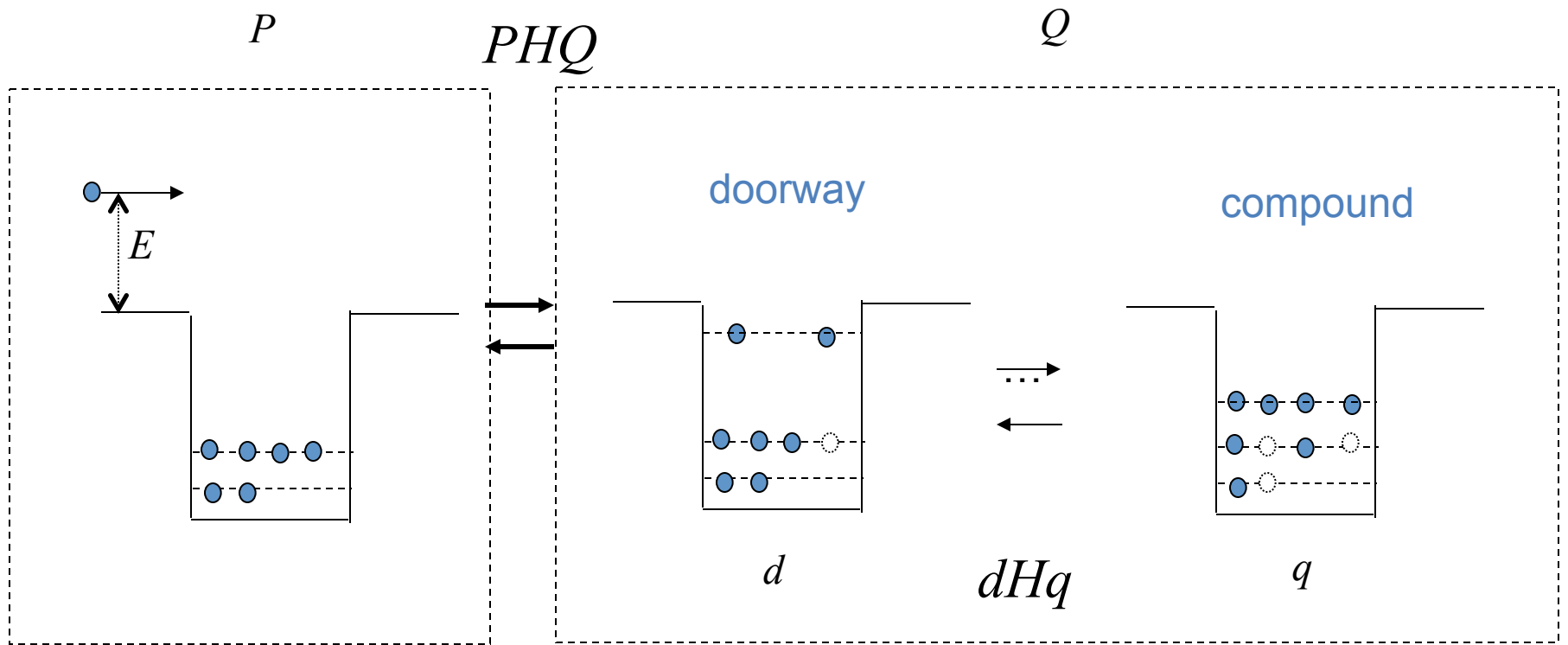
Year 5 Progress Report

- **Year 5 Reaction Deliverable #55:**
 - “Examine energy-dependence of eigensolutions in the expansion for the KKM theory.”
- **Year 5 Progress Report:**
 - **Prototyped energy dependence in KKM:**
 - Intel MKL implementation of complex symmetric eigensolver on 12 cores
 - **Massively parallel code in “ensemble” eigensolver of complex symmetric matrices (K. Roche).**
 - In the meantime: loop through energies on the parallel code.
- **Related HPC contribution:**
 - **Massively Parallel eigensolver for large (ensembles) of complex symmetric matrices**

Why KKM?

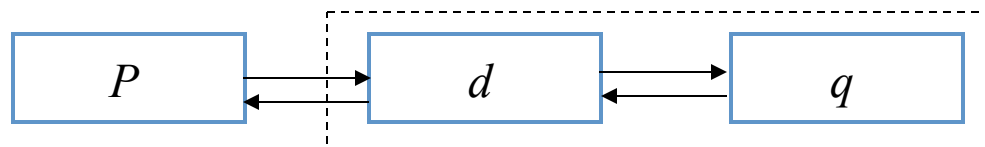
- A framework based on Feshbach's projection operators
- Central result:
 - $T = T_{\text{background}} + T_{\text{resonant}} = T_{\text{average}} + T_{\text{fluctuating}}$
- A foundation for derived statistical theories:
 - Kerman-McVoy
 - Designed for two step processes like $A(d,p)B^*$, $B^* \rightarrow A+n$
 - Could be used for statistical (d,p) reactions at FRIB
 - Feshbach-Kerman-Koonin (FKK)
 - Multistep reactions, used for nuclear data analysis
- Similar expressions were derived later by other methods

Physical picture



continuum

bound



Feshbach's projection operators

$$H\Psi = E\Psi$$

$$P + Q = 1 ; \quad P \cdot Q = 0 \quad P^2 = P \quad H_{PQ} \equiv PHQ$$

$$(E - H_{PP})P\Psi = H_{PQ}\Psi$$

$$(E - H_{QQ})Q\Psi = H_{QP}\Psi$$

$$(E - H_{PP})\chi = 0$$

Two-potential formula yields

$$\begin{aligned} \Rightarrow T &= \langle \phi | V_{PP} | \chi \rangle + \langle \chi | H_{PQ} \frac{1}{E - H_{QQ} - H_{QP} \frac{1}{E - H_{PP}} H_{PQ}} H_{QP} | \chi \rangle \\ &\equiv T_{\text{background}} + T_{\text{resonant}} \end{aligned}$$

KKM subtraction

Kawai, Kerman, and McVoy
Ann. of Phys. 75, 156 (1973)

$$(E - H_{PP})P\Psi = H_{PQ}\Psi \quad (1)$$

$$(E - H_{QQ})Q\Psi = H_{QP}\Psi \quad (2)$$

$$Q\Psi = \frac{1}{E - H_{QQ}}H_{QP}\Psi$$

$$(E - H_{PP})P\Psi = H_{PQ} \frac{1}{E - H_{QQ}} H_{QP} P\Psi$$

$$(E - H_{\text{opt}})\overline{P\Psi} = 0$$

$$H_{\text{opt}} \equiv H_{PP} + H_{PQ} \frac{1}{E - H_{QQ} + iI} H_{QP}$$



(3)
Energy averaging of
the T-matrix yields this
expression for optical
potential and opt.wave-f.
(for Lorentzian averaging)

$$(E - H_{\text{opt}})P\Psi = H_{PQ} \left(\frac{1}{E - H_{QQ}} - \frac{1}{E - H_{QQ} + iI} \right) H_{QP} P\Psi$$

Use H_{opt} to
rewrite Eq. (3)

$$= H_{PQ} \sqrt{\frac{iI}{E - H_{QQ} + iI}} \frac{1}{E - H_{QQ}} \sqrt{\frac{iI}{E - H_{QQ} + iI}} H_{QP} P\Psi$$

$$\equiv V_{PQ} \frac{1}{E - H_{QQ}} V_{QP} P\Psi$$

KKM Fluctuation T-matrix

$$\begin{aligned} (E - H_{\text{opt}})P\Psi &= V_{PQ}\Psi \\ (E - H_{QQ})Q\Psi &= V_{QP}\Psi \\ (E - H_{\text{opt}})\overline{P\Psi} &= 0 \end{aligned}$$

Two-potential formula yields

$$\begin{aligned} \Rightarrow T &= \langle \phi | H_{\text{opt}} | \overline{\Psi} \rangle + \langle \overline{\Psi} | V_{PQ} \frac{1}{E - H_{QQ} - V_{QP} \frac{1}{E - H_{\text{opt}}} V_{PQ}} V_{QP} | \overline{\Psi} \rangle \\ &\equiv T_{\text{optical}} + T_{\text{fluctuation}} \end{aligned}$$

$$\Rightarrow \langle T_{\text{fluctuation}} \rangle \approx 0$$

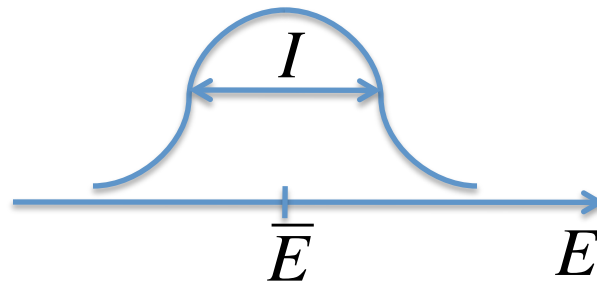
$$\Rightarrow \langle \sigma \rangle \approx \sigma_{\text{optical}} + \langle \sigma_{\text{fluctuation}} \rangle$$

Expand the T-matrix by eigenfunctions

$$T_{cc'}^{\text{fluct}}(E) \equiv \frac{1}{2\pi} \sum_q \frac{g_{cq}(E)g_{c'q}(E)}{E - \mathcal{E}_q(E)}$$

$$g_{cq}(E) = \sum_Q \langle \psi_c(E) | V_{cQ}(E) | Q \rangle \langle Q | q(E) \rangle$$

This E-dependence now treated explicitly.

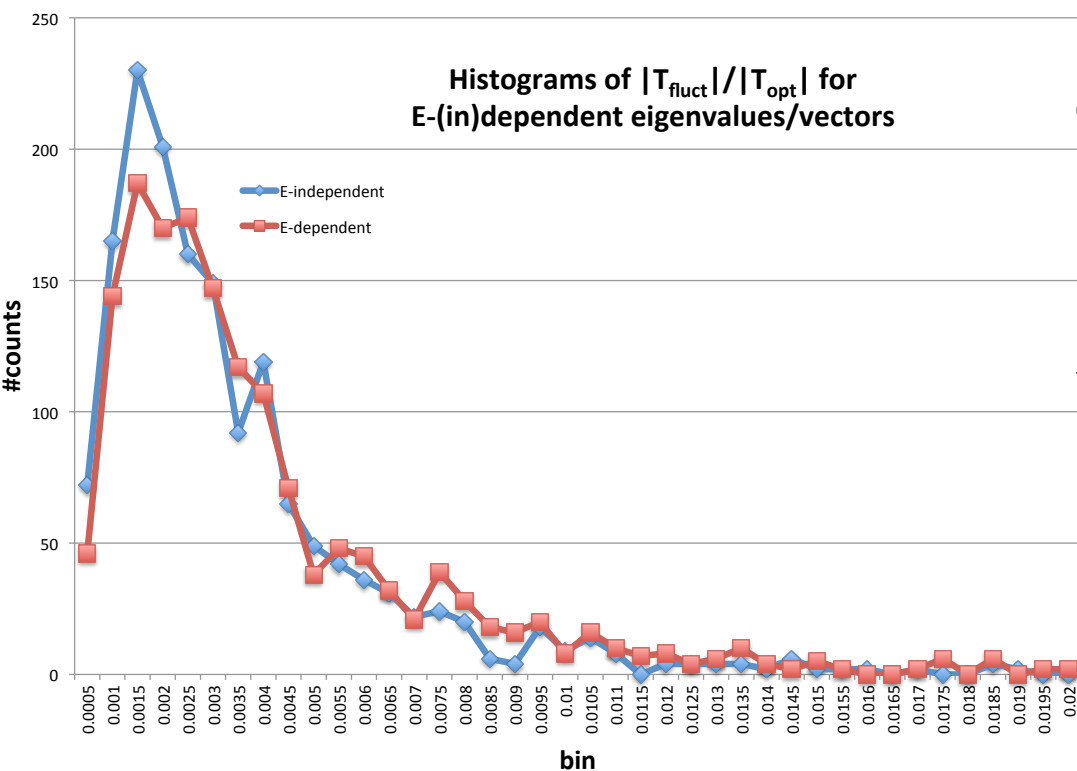


Lorentzian weight function width I .

$$\langle T_{cc'}^{\text{fluct}}(E) \rangle_I \equiv \frac{I}{2\pi} \int \frac{dE'}{(E - E')^2 + \frac{I^2}{4}} T_{cc'}^{\text{fluct}}(E')$$

Preliminary Results:

Eigenvalues/vectors	Average Ratio	SQRT(Variance)
E-independent	0.0037	0.0053
E-dependent	0.0042	0.0049



Computation parameters:

- Eigenvalues/vectors computed at 100 energies spanning 18-22 MeV
- 1600 equidistant Q-levels
- 40 channels
- 20 equidistant radial points where H_{PQ} set to a Gaussian-distributed random interaction
- $E = 20$ MeV
- 100 E' points for Lorentzian averaging between 18 and 22 MeV
- Lorentzian averaging width $\Gamma = 0.5$ MeV
- s-wave only
- Strongly overlapping resoances

Test approximations in KKM derivation

- The E-dependence makes E-averaging more accurate

$$T_{cc'} = \bar{T}_{cc'} + \frac{1}{2\pi} \frac{g_{qc}(E)g_{qc'}(E)}{E - \mathcal{E}_q(E)} = \bar{T}_{cc'} + T_{cc'}^{\text{fluct}}$$

$$\Rightarrow \langle \sigma_{cc'}^{\text{fluct}} \rangle \sim \left\langle \left| T_{cc'}^{\text{fluct}} \right|^2 \right\rangle_I$$

$$\cong \left\langle \sum_q \frac{g_{qc}g_{qc'}}{E - \mathcal{E}_q} \frac{g_{qc}^*g_{qc'}^*}{E - \mathcal{E}_q^*} \right\rangle_I$$

$$\cong 2\pi \left\langle \frac{g_{qc}g_{qc'}g_{qc}^*g_{qc'}^*}{D_q\Gamma_q} \right\rangle_q$$

$$\cong \frac{2\pi}{D_q\Gamma_q} \left\langle g_{qc}g_{qc'}g_{qc}^*g_{qc'}^* \right\rangle_q$$

$$\cong X_{cc'}X_{c'c'} + X_{cc'}X_{c'c}$$



Random Phase Hypothesis

Preliminary results are analyzed.

where

$$X_{cc'} \equiv \left(\frac{2\pi}{D\Gamma} \right)^{1/2} \left\langle g_{qc}g_{qc'}^* \right\rangle_q$$

HPC progress report (by K. Roche)

- implemented novel parallel complex symmetric diagonalization routine in the spirit of ScaLAPACK
 - requires more extensive testing at scale
 - tested against zgeev()
 - self-consistent tests (|AZ-DZ|) (n= 65536)
 - against Toeplitz form (n=32768)
- implementation of triangular solves are one bottleneck that can be improved
- remove the kfil() data structures -stay incore
- plug in the parallel , parallel diagonalization routines over energies -code exists but we have not tested it
 - $E \sim E_1, E_2, \dots, E_n$
 - instead of doing these in sequence, do them at once
 - form at most n subcommunicators of size $P*Q$; ($np \sim n * P * Q$)
(P, Q are dimensions of virtual rectangular process grid)
 - perfect strong scaling over diagonalization phase in simple tests

Year 5 plan

- Complete *parallel* KKM with E-dep. eigenvalues/vectors
- Test approximations in derivation of KKM cross sections
- Publish the KKM work (including the work on doorways)