# Theory Initiatives

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NC State

Task: Discuss progress on theory Initiatives since the 2015 Long Range Plan

# LRP Theory Initiatives

- New investments in computational nuclear theory
- Establish FRIB Theory Alliance
- Increase the number of topical collaborations

Endorsement: Develop plan to enhance theory effort in neutrinos and fundamental symmetries

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# Computational Nuclear Theory

We recommend new investments in computational nuclear theory that exploit US leadership in high-performance computing. These new investments include a timely enhancement of the nuclear physics contribution to SciDAC and complementary efforts as well as deployment of the necessary capacity computing.

# Computational Nuclear Theory: SciDAC

What? SciDAC funds personnel that use existing machines for scientific goals.

By whom? SciDAC funding is currently roughly ½ NP and ½ ASCR.

Status? Third round of this program is ending in August. DOE FOA for SciDAC-4, proposals collected and reviewed.

Awaiting funding announcement …

# Computational Nuclear Theory: Complementary Efforts

NP community wrote an extensive white paper on exascale computing.

What? ECP (Exascale computing) This funding is to develop codes that can make use of exascale architecture when exascale machines arrive.

By whom? funded by ASCR

Status? awarded 15 full & 7 seed projects.

Two awards in NP since LRP:

Exascale lattice gauge theory (full, with HEP)

Exascale models of stellar explosions (seed)

# Computational Nuclear Theory: Complementary Efforts

What? JETSCAPE develops codes for jet physics in heavy ion collisions.

By whom? The SI2 program (NSF Office of Advanced Infrastructure, Physics Division, Division of Mathematical Sciences)

Status? Awarded last year

# Computational Nuclear Theory: Capacity Computing

Capacity computing addresses intermediate scale computing needs. Many nuclear theorists need more than a few workstations but less than a capability machine, or use clusters for analysis/post-processing.

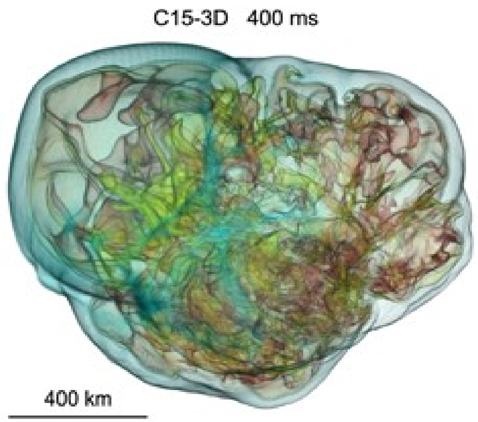
Most organized current hardware effort is in Lattice QCD:

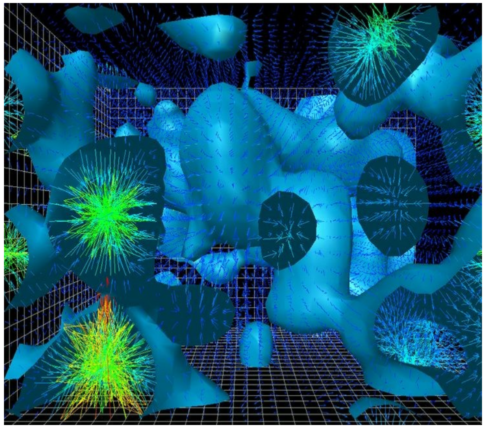
What? LQCD-ext II

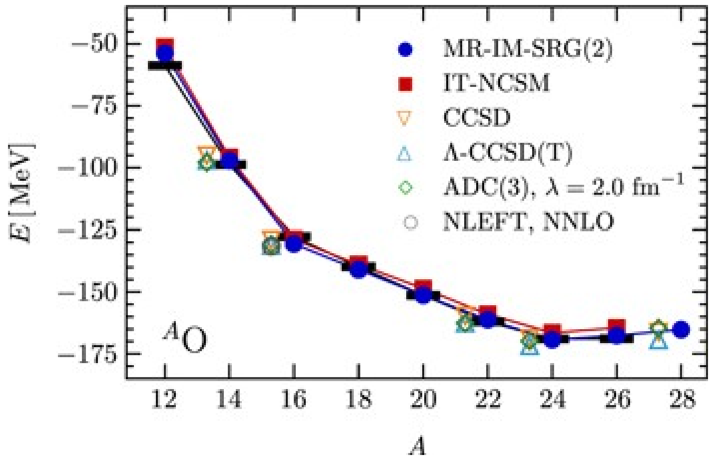
By whom? DOE HEP and NP

Status? Ending in FY19, contemplating next round

# Computational Nuclear Theory: Some Examples






Top left: Core collapse supernova simulation.
Top right: Lattice QCD calculation of gluon fields.
Bottom left: Nuclear structure calculations of binding energies of oxygen isotopes using ab-initio methods.
Many more examples ...

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# FRIB Theory Alliance

We recommend the establishment of a national FRIB Theory Alliance. This distributed network will enhance the field through the national FRIB theory fellow program and tenure-track bridge positions at universities and national laboratories across the U.S.

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

# FRIB Theory Alliance

- Purpose: foster advancements in theory related to diverse areas of FRIB science.  Charter ratified April 2016.
- Theory alliance board has shown lots of activity – significant infrastructure in place in terms of plans, committees and procedures.
- Highlight: introduction of a National FRIB Theory Fellow program with a fellow placed at LANL
- Proposal submitted in October for expansion of program - previous project period was 2 FRIB theory fellows supported at 50%.
- Status: funding for the second project period has been recommended by the Office of Science.  Plan is to increase number of theory fellows and initiate the faculty bridge position program.

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# Topical Collaborations

We recommend the expansion of the successful Topical Collaborations initiative to a steady-state level of five Topical Collaborations, each selected by a competitive peer-review process.

Pre-LRP: Three topical collaborations (Neutrinos and Nucleosynthesis, JET, TORUS), all have now ended.

Current status: Four new collaborations are funded, slightly under 500K/year.

TMD collaboration
BEST collaboration
DBD collaboration
FIRE collaboration

All funded by DOE NP, FIRE collaboration is jointly funded with NNSA/NA221.

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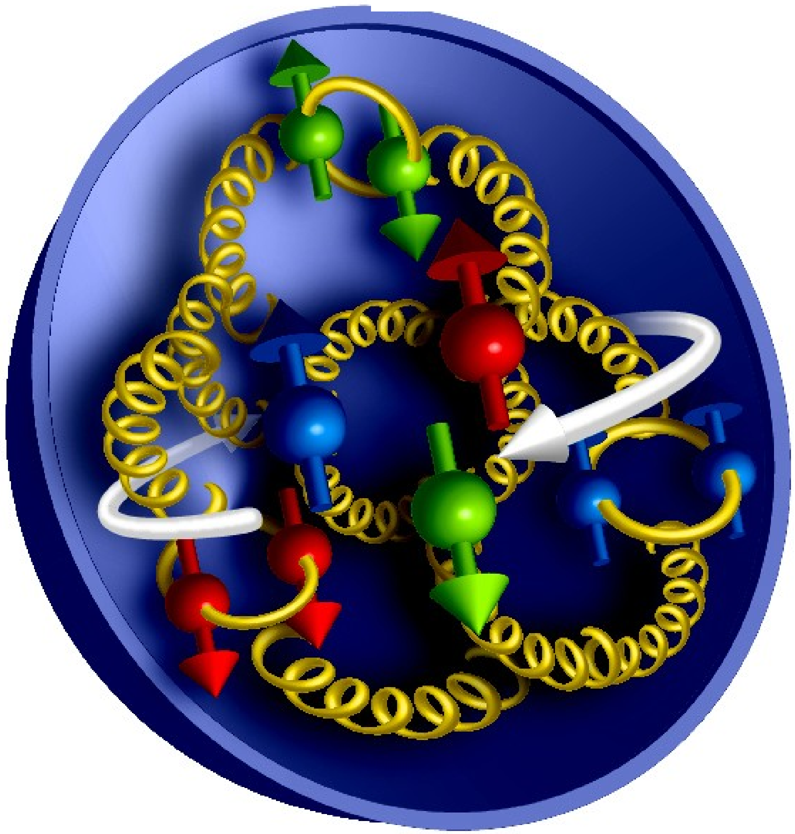
# TMD Collaboration



- Overarching goal: a 3D picture of the nucleon
- To go beyond 1D-parton distributions requires TMDs Transverse Momentum Distributions
- Developing and fitting TMDs for broad use requires an organized theory effort

TMD Collaboration

# Strategy

1) Theory of TMDs: Study definitions, universality

2) Lattice determination of TMDs.

3) Global fits to experimental observables.

4) Combine all three for internal picture of nucleon

5) Applications: Interpretation of experiments, study observables for EIC

TMD Collaboration

- 14 institutions
- Started Spring 2016
- Highlight: summer school on hadron structure to run in June, 30 students
- Two faculty bridge positions: one filled at Temple, one search in progress at New Mexico State
- Partial students and postdocs funded

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# Beam Energy Scan Theory

BEST COLLABORATION

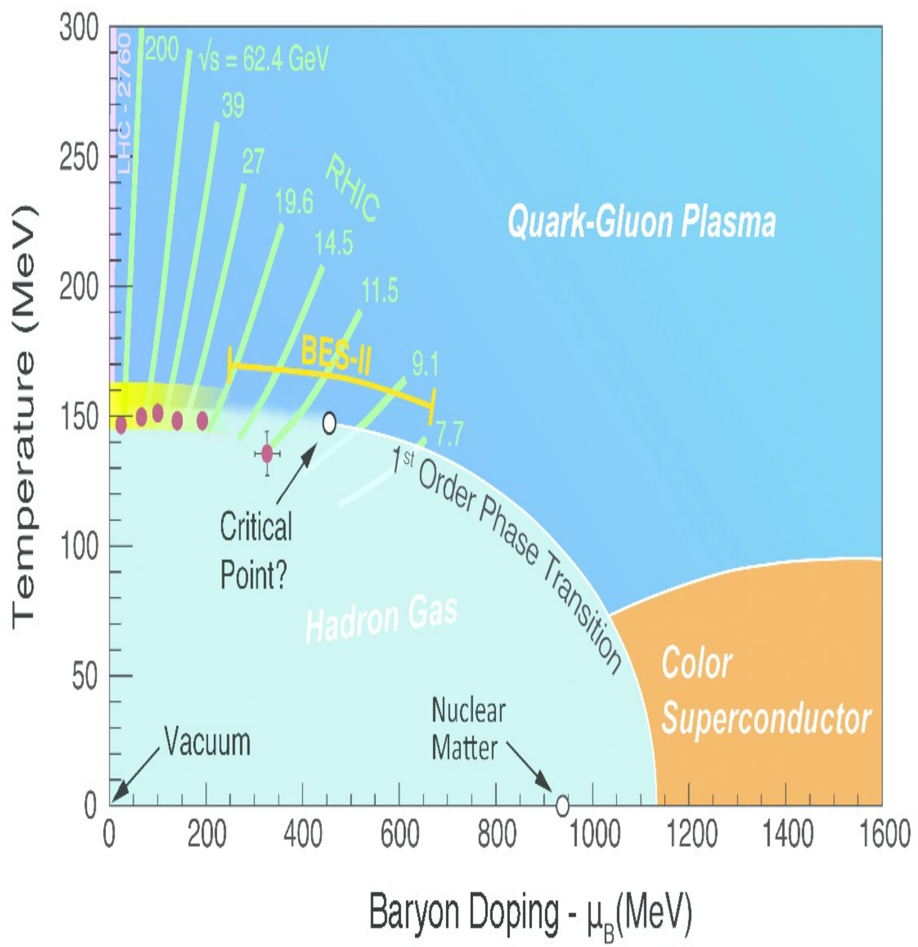
- 12 institutions
- Two faculty bridge positions, searches ongoing.
- Student, postdoc support
- Started Spring 2016

Experimental Beam Energy Scan program: run RHIC at a series of energies below top energy

With a concerted theory effort, two major discoveries may be possible:

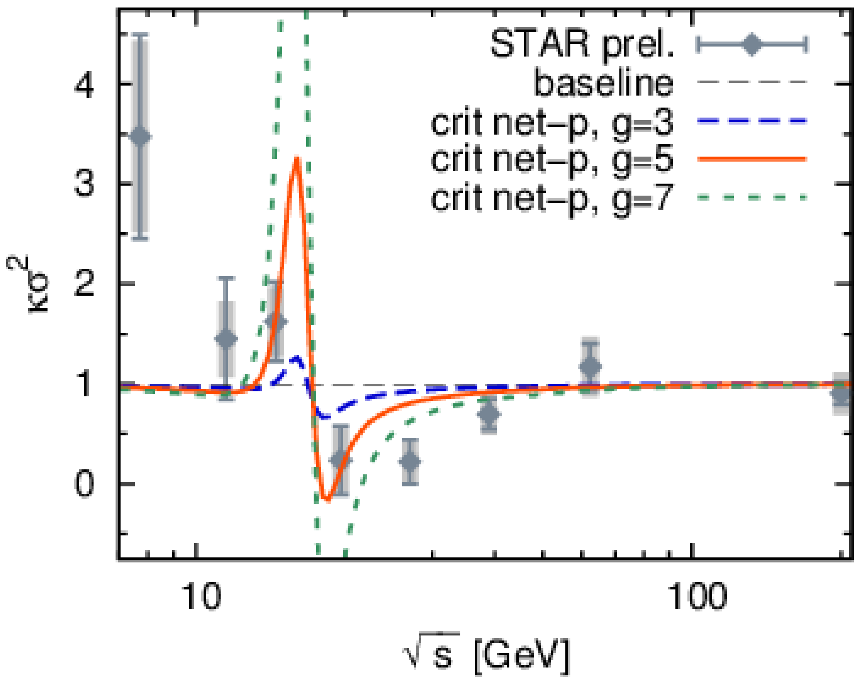
- Critical point in the QCD phase diagram
- Anomalous chiral magnetic effect (CME)

# BEST: Critical Point




- Critical point, past which there is a discontinuous transition from the QGP to hadrons, is proposed, but not yet seen experimentally
- Collaboration will provide predictions for or interpretation of fluctuation (and CME) observables

# BEST: Critical Point Highlight




- Objective: Compare theory directly with experiment
- Fluctuation observable is plotted against beam energy
- At the critical point expect large fluctuations, which manifest themselves in dramatic behavior of  fluctuation observable
- Idea: Predictions become more sophisticated while experiment becomes more accurate and fills in critical region.

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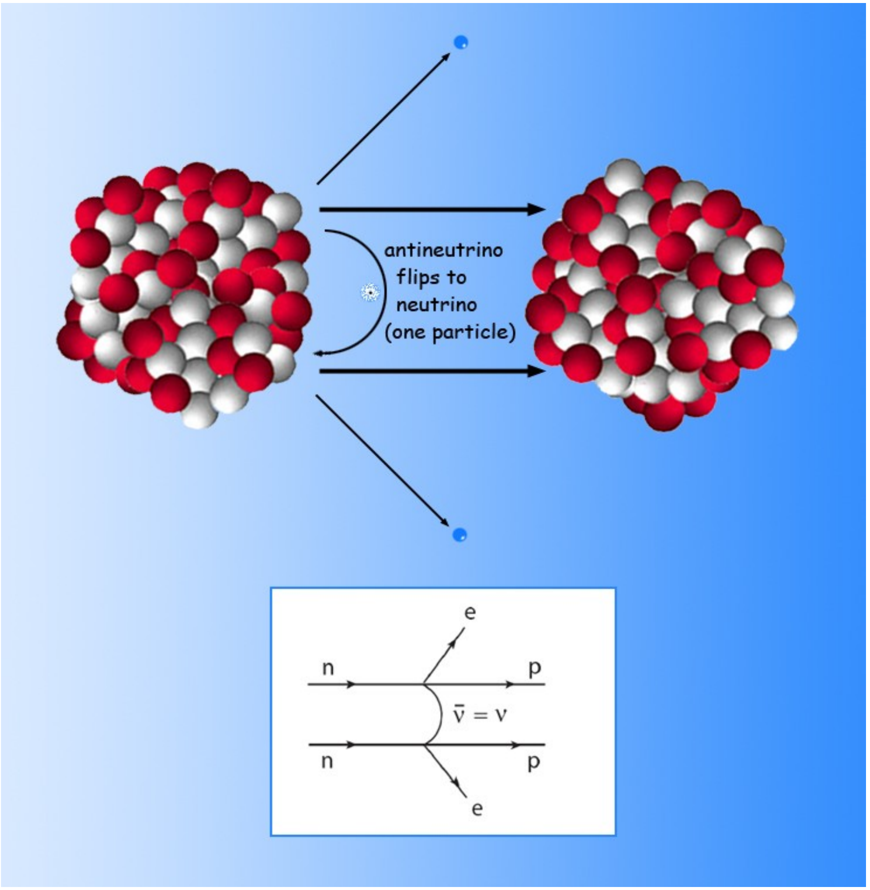
# Nuclear Theory for Double Beta Decay and Fundamental Symmetries: DBD collaboration




Neutrinoless double beta decay experiments require matrix element information in order to interpret their result in terms of neutrino mass.

Other fundamental symmetries experiments, e.g. nuclear and atomic electric dipole moments, similarly require input from nuclear structure.

# DBD Collaboration

- Started Spring 2016
- Ten institutions
- Two bridge positions: one filled at UNC, search planned at Iowa State
- Also supports postdocs/students

Idea: In past nuclear properties were determined by fitting model parameters to other properties in same region. Theoretical predictions of $0\nu$ double beta decay matrix elements had large variations.

This collaboration will apply new ab-initio methods in nuclear structure to DBD.

Main deliverable: More accurate calculations for DBD with reliable error bars

# DBD Collaboration Highlight

Full Chiral NN + NNN Calculation (Preliminary)

From G. Hagen

| Method | $E3_{max}$ | $M^{0\nu}$ |
|---|---|---|
| CC-EOM (2p2h) | 0 | 1.23 |
| CC-EOM (3p3h) | 10 | 0.33 |
| CC-EOM (3p3h) | 12 | 0.45 |
| CC-EOM (3p3h) | 14 | 0.37 |
| CC-EOM (3p3h) | 16 | 0.36 |
| SDPFMU-DB | - | 1.12 |
| SDPFMU | - | 1.00 |

Preliminary

Last two are two-shell shell-model calculations with effective interactions.

Coupled cluster calculation based on ChiPT.

Observation: As you increase from 2p-2h to 3p-3h the value for the matrix elements begins to diverge significantly from shell model calculations that use effective interactions.

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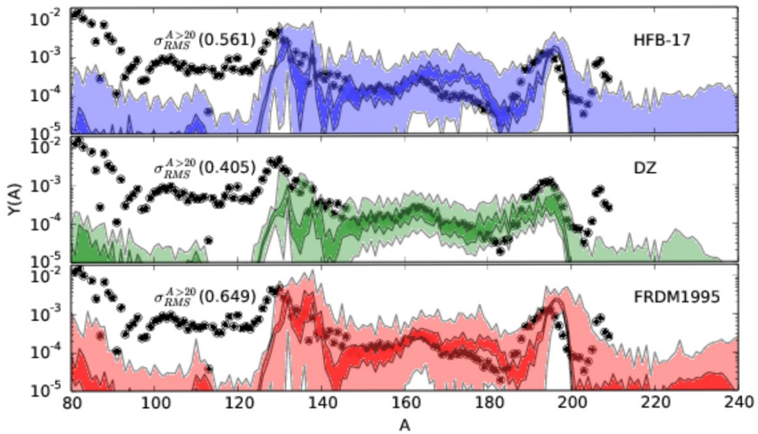
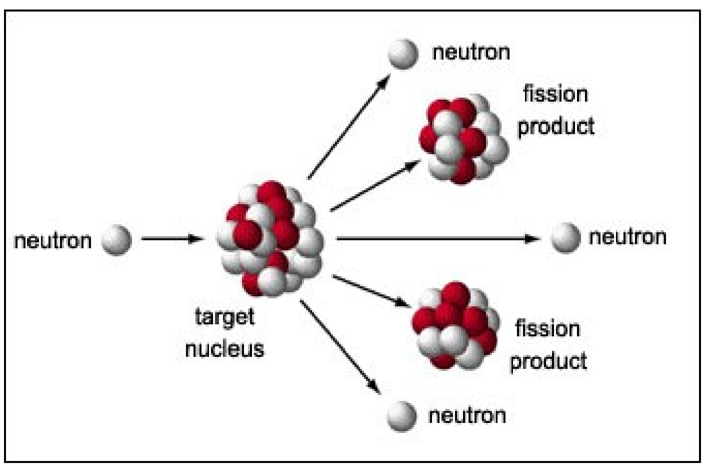
# Fission in r-Process Elements: FIRE Collaboration




The search for the astrophysical site of the r-process elements is complicated by uncertainties in nuclear physics inputs




Fission rates and daughter products of interest to the r-process are hard to explore experimentally, but are absolutely crucial to comparing predicted abundance yields to data.

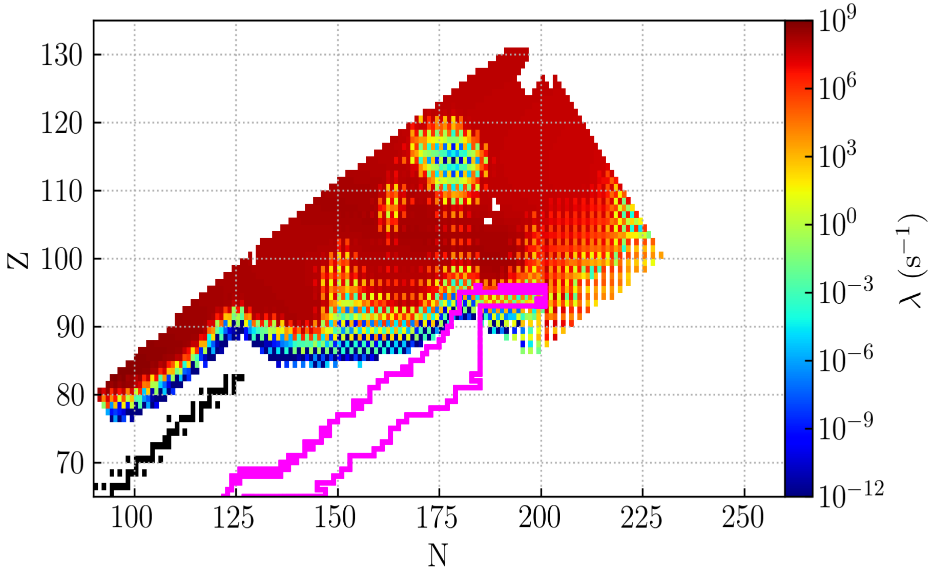
# FIRE Collaboration

- Started Fall 2016
- Five institutions
- Funds primarily postdocs, students, researchers at national laboratories
- Leverages the combined expertise of fundamental nuclear theory, nuclear data from phenomenological models, management and applications of nuclear data and astrophysical simulation.

Deliverables:

- Computation of fission rates and yields.
- Systematic implementation of fission rates and yields in r-process models, including neutron induced, beta delayed and spontaneous fission.
- Fission database

# FIRE Collaboration: Recent Highlight




- Figure shows neutron induced fission rates calculated by the collaboration at a snapshot in the r-process.
- Pink region shows the r-process path. Indicates neutron induced fission is a potential termination mechanism for the path.

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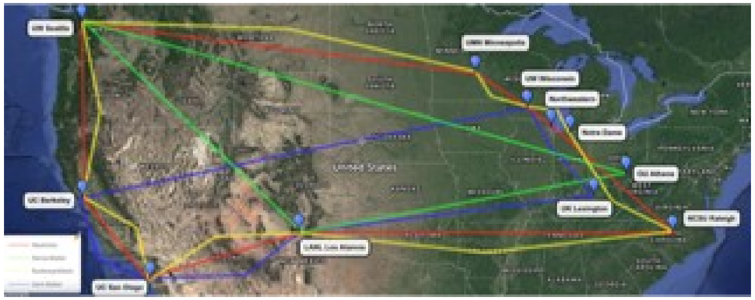
# Endorsement: Strategic plan to enhance theory effort in neutrinos and fundamental symmetries

The community endorses undertaking a development and initiation of a strategic plan to address the need for an enhanced theoretical effort and sustained theory-experiment interactions in the area of fundamental neutrinos and symmetries.

Progress in two areas: DBD collaboration (already discussed) and NSF Hub

# NSF Hub: Network in Neutrinos, Nuclear Astrophysics and Symmetries - N3AS



Multi-institution effort to train postdoctoral fellows and advance research in neutrinos, dense matter, dark matter and fundamental symmetries

Funding level similar to topical collaborations

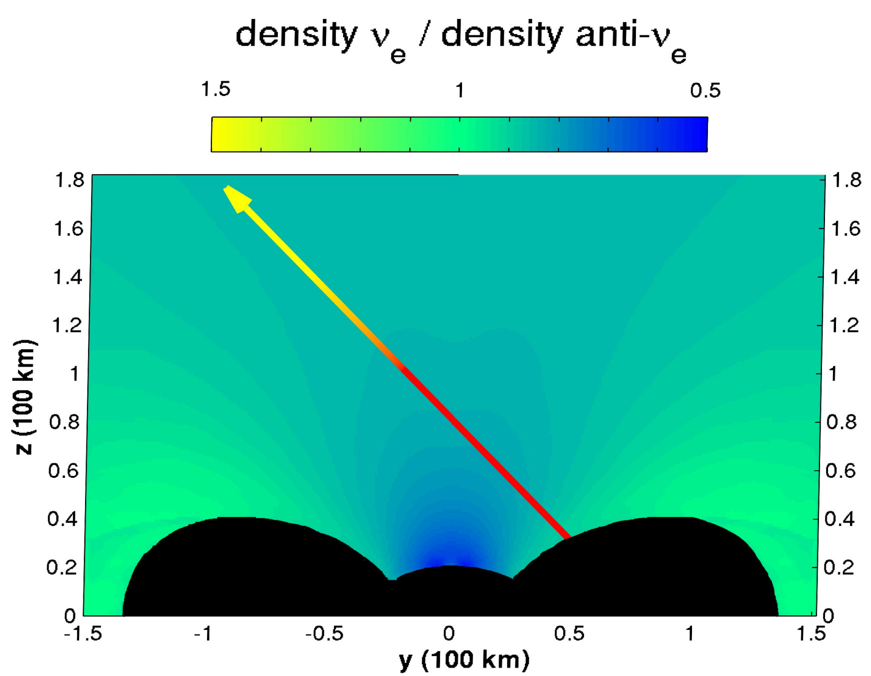
N3AS started in Fall 2016

Eight postdoctoral fellows will be hired in the collaboration's five year period

Nuclear physics of multi-messenger signals from neutron star mergers and supernovae. Neutrino signals, gravitational waves, electromagnetic signatures and r-process abundances → this provides valuable input into 1) dense matter and 2) neutrino physics 3) origin of the elements.

Nuclear physics of 3) dark matter. How dark matter detection limits, dark matter simulations and astronomical observation enhance our understanding of nuclear physics.

- Highlight: Three postdoctoral fellows hired and will start in Fall 2017



# (Too soon to draw) Conclusions

- SciDAC-4: Awaiting award announcements
- ECP: One full (with HEP), one seed project
- SI2: One award
- FRIB theory initiative: Infrastructure being developed, recommended for funding.
- Topical collaborations: Four awards
- NSF theory hub in neutrinos & fundamental symmetries awarded.