Data mining the EXFOR database

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5-8 November 2013, Geel, Belgium

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery

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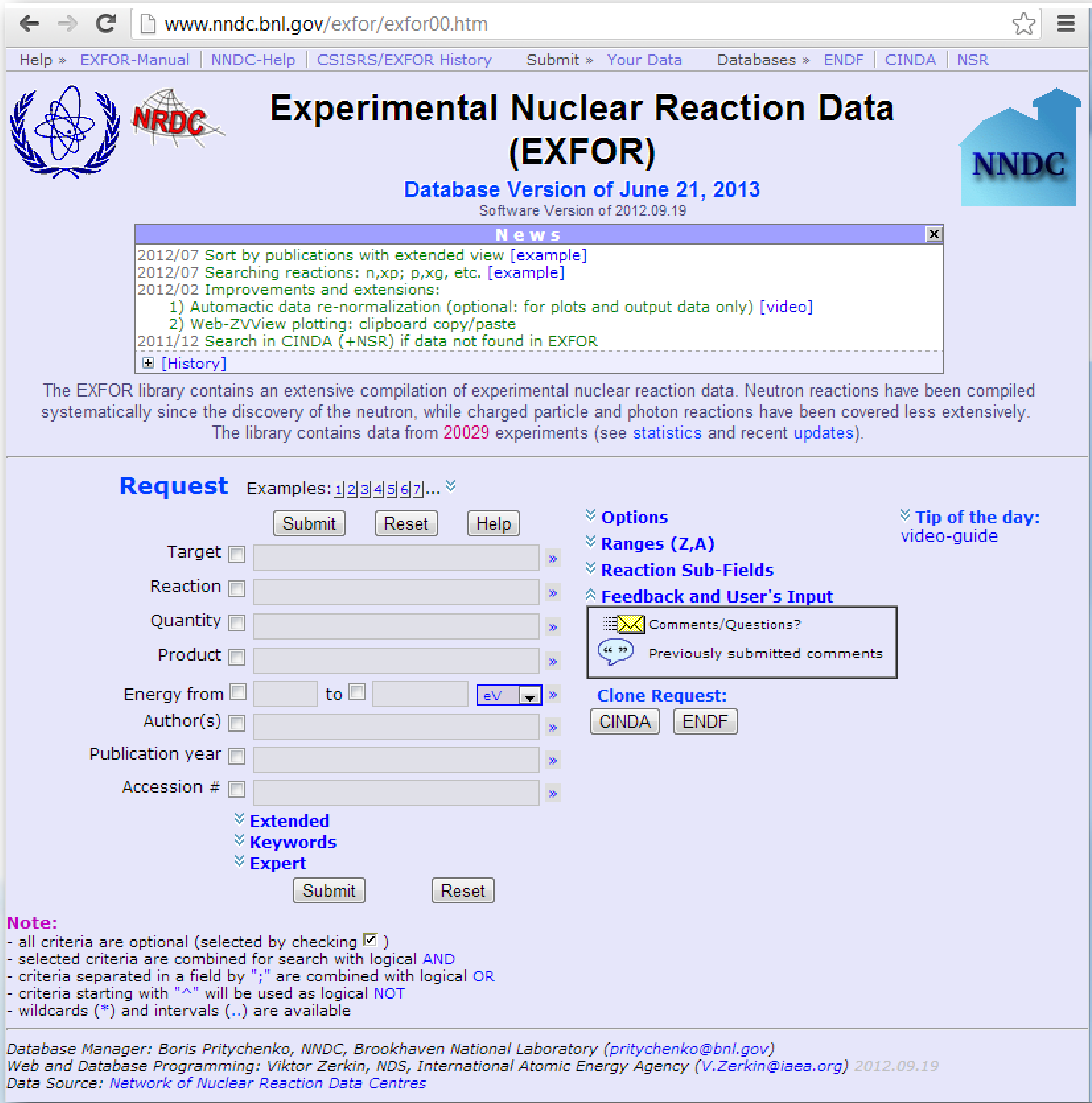
The EXFOR library contains nearly all experimental nuclear results



- Data from ~ 20,000 experiments
- Earliest experiments from 1935
- Most complete compilation of experimental nuclear data
- Mostly *n*-induced, but lots of CP-induced, photonuclear and other data

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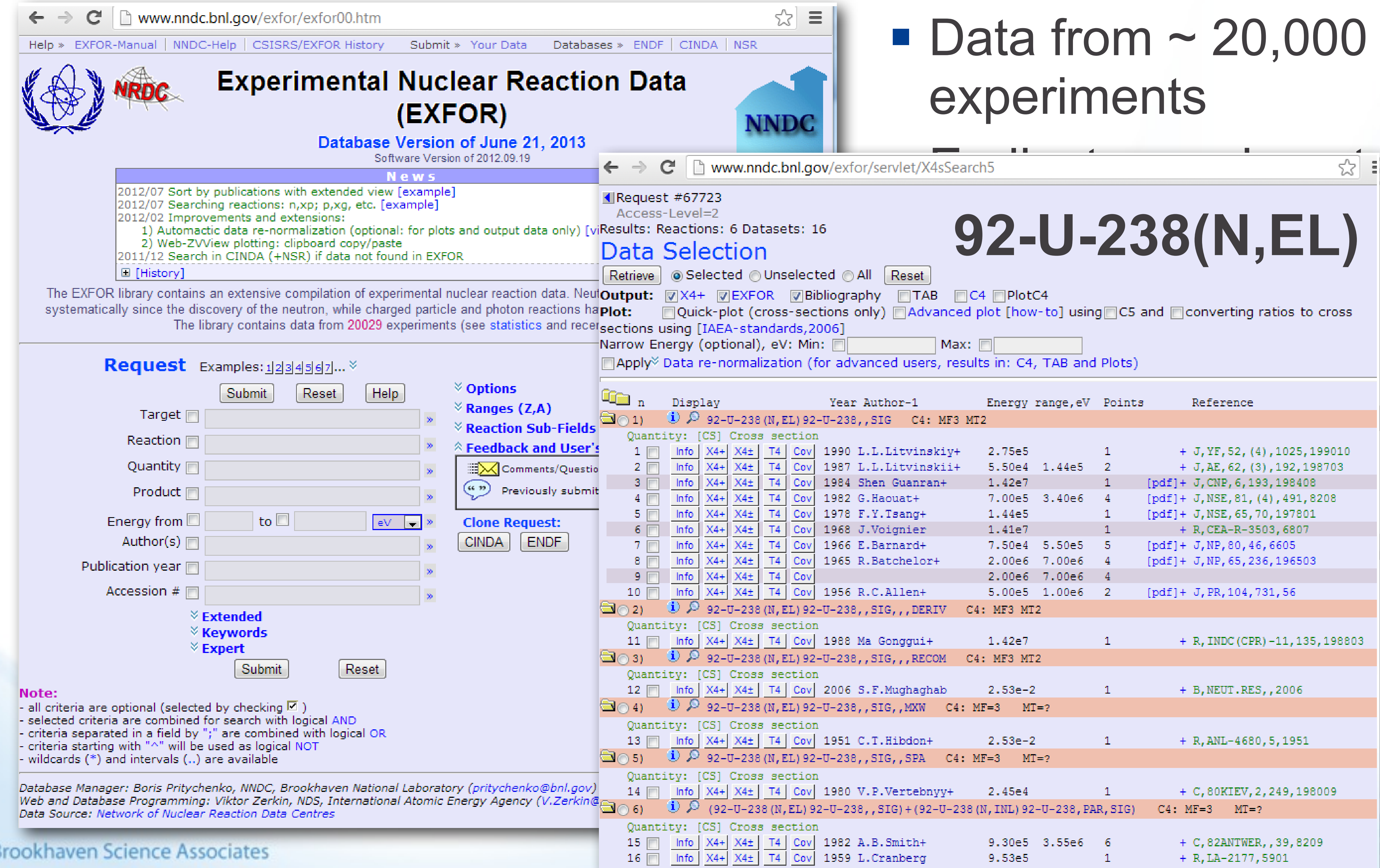

- Data from ~ 20,000 experiments

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SUBENT        11135001     860905              20050926       0000
BIB                  6         10
INSTITUTE  (1USACOL)
REFERENCE  (J,PR,60,702,4111)
           (J,PR,58,1004,40) COMMENT ON SPECTRUM.
AUTHOR     (H.CARROLL,J.R.DUNNING)
TITLE      THE INTERACTION OF SLOW NEUTRONS WITH GASES.
STATUS     (SCSRS)
HISTORY    (760628T) TRANSLATED FROM SCISRS
           (820108A) CONVERTED TO REACTION FORMALISM
           (840217A) REFERENCE CORRECTED.
           (860905A) ENERGY MOVED TO SAN 1.
ENDBIB              10
COMMON               1          3
EN-DUMMY
EV
 0.0253
ENDCOMMON            3
ENDSUBENT           17
SUBENT        11135009     860905              20050926       0000
BIB                  3         12
REACTION   (1-H-1(N,TOT),,SIG,,MXW)
SAMPLE     H2O LIQUID
           AUTHOR ALSO GIVES DATA FOR 10 OTHER SAMPLES -
                H-2 GAS       - 31.8+-0.5 B
                CH(4) GAS     - 45.4+-0.3 B
                C(2)H(6) GAS  - 46.4+-0.5 B
                C(3)H(8) GAS  - 46.9+-0.6 B
                C(4)H(10) GAS - 48.7+-0.6 B
                PARAFFIN      - 49.8+-0.2 B
                DOTRIACONTANE - 50.2+-0.2 B
HISTORY    (780914C)
           (860905A) REACTION CORRECTED.
ENDBIB              12
NOCOMMON             0          0
DATA                 2          1
DATA       DATA-ERR
B          B
 44.6       0.5
ENDDATA              3
ENDSUBENT           20
ENDENTRY             2
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ENTRY 11135

Carroll & Dunning "Interaction of slow neutrons with gases" from Physics Reports 1941

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REACTION (1-H-1(N,TOT),,SIG,,MXW)

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This is 9th subentry on ^{1}H scattering

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The data is one spectrum averaged point

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REACTION & MONITOR fields denote what reaction/quantity measured

- **EXFOR REACTION fields and MONITOR fields have essentially the same format**
  - REACTION denotes what is measured
  - MONITOR denotes what the REACTION is measured “relative” to
- **For a simple measurement:**

```
(1-H-1(N,TOT),,SIG,,MXW)
```

Reaction studied (1-H-1(N,TOT))

Quantity measured (SIG,,MXW)

REACTIONs & MONITORs have complicated variants

- **Mathematical relations in REACTIONs and MONITORs**:
  - Reaction combinations:

    ```
    (3-LI-6(N,T)2-HE-4,,SIG,,SPA)/(92-U-235(N,F),,SIG,,SPA)
    ```

    any relation using +,-,*,/,//,= allowed
  - “Isomer math”:

    ```
    (72-HF-177(N,G)72-HF-178-M/T,,SIG/RAT)
    ```
- **Several reactions/quantities have special meanings**:
  - ALF: capture-to-fission ratio
  - ETA: ave. neutron yield per nonelastic event for *n*-induced reactions
  - RI: resonance integral
  - NON, INEL, SCT: all obey sum rules
- **Elemental data**
  - weighted average of reaction on isotopes comprising element

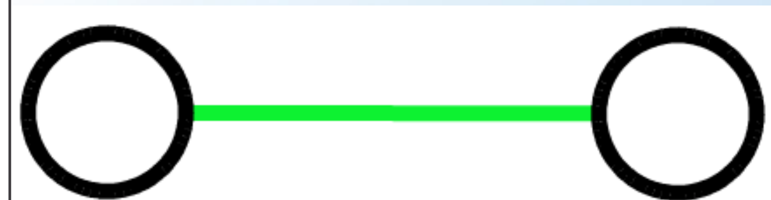
These variants encode connections between simple REACTIONs

Can we learn anything just looking at the REACTIONs and MONITORs alone?

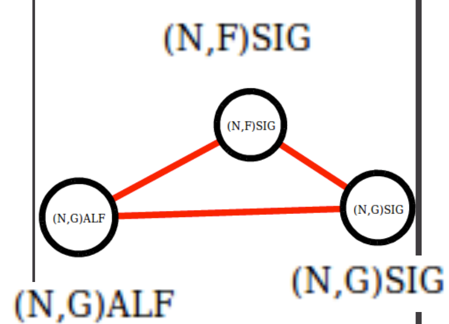
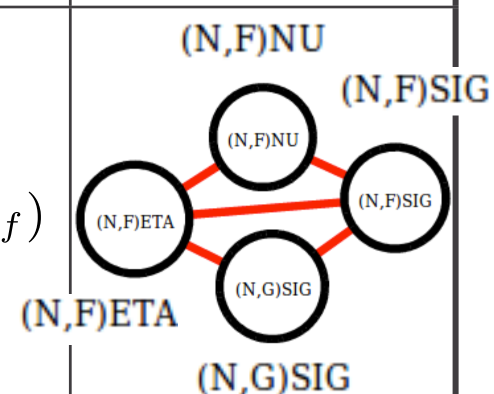
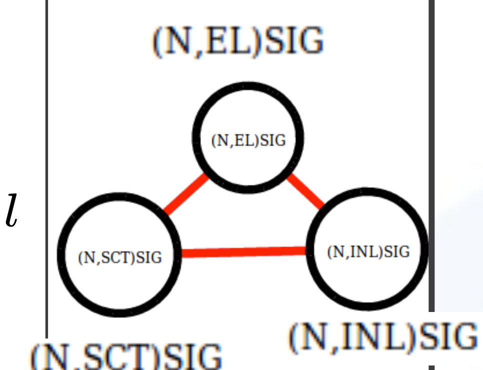
Types of nodes

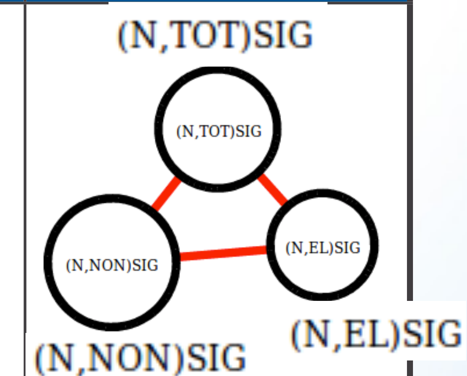
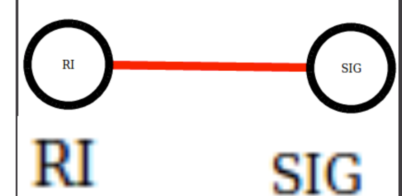
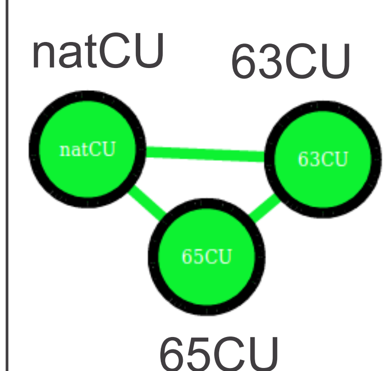
Description	Example
Regular node	
CIELO isotope Chadwick, M., "CIELO: A Future Collaborative International Evaluated Library", Proc. of the International Conference of Nuclear Data for Science and Technology (ND2013)	
ENDF/B-VII.1 Standards Carlson A.D. "International Evaluation of Neutron Cross Section Standards", Nuclear Data Sheets. 110.12 (2009) 3215-3324.	
Standards proposed at IAEA Technical Meeting, July '13	
Standards proposed in the past / Proposed by us	
Mughabghab, S. F., *Atlas of Neutron Resonances*, Elsevier Science, April 17, 2006.	
Diagnostic radioisotopes and monitor reactions P. Oblozinsky, International Atomic Energy Agency IAEA, IAEA-TECDOC-1211 http://www-nds.iaea.org/medical/	
Isomer target	
Elemental target	

Types of connections

Edge type	Description	Example
MONITOR	Typically a, well characterized reaction used to reduce or eliminate systematic experimental errors.	
Mathematical relation (e.g. “isomer math”; sum rules; math is REACTION string; ALF, ETA, etc)	Connections representing a simple ratio or a more complex mathematical equation.	
Neutron Standards/ CIELO	All evaluated simultaneously and therefore are linked.	
Elemental	Data on a elemental target is connected to every stable isotope of the element for the same measurement.	

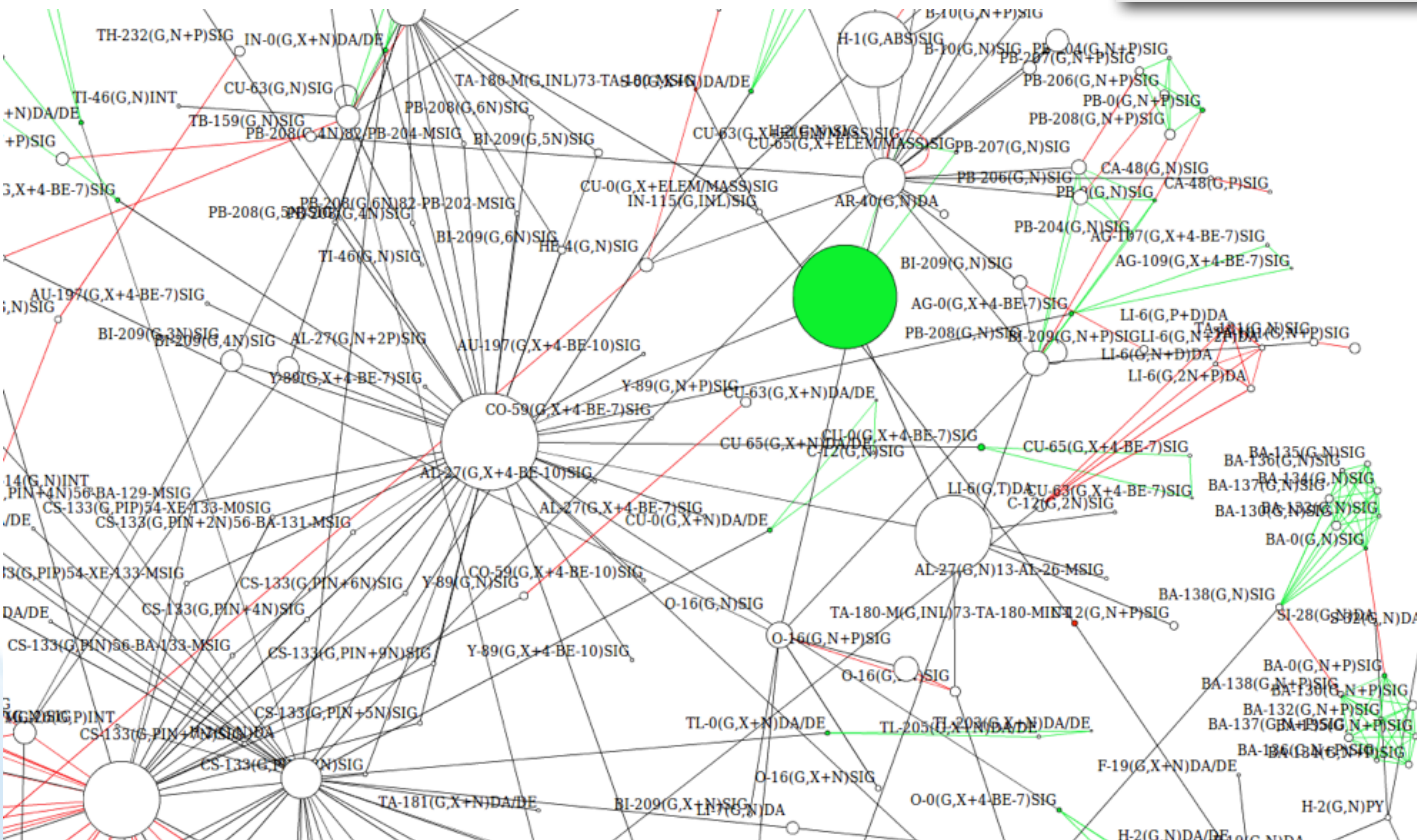
Reoccurring motifs

EXFOR Quantity	Definition	Example
ALF	σ_γ / σ_f	
ETA	$\overline{\nu}\sigma_f/(\sigma_\gamma + \sigma_f)$	
SCT	$\sigma_{el} + \sigma_{inel}$	

EXFOR Quantity	Definition	Example
NON	$\sigma_{tot} - \sigma_{el}$	
RI	$\int_0^\infty dE \frac{\sigma(E)}{E}$	
(elemental)	$\sum_i w_i \sigma_i(E)$	

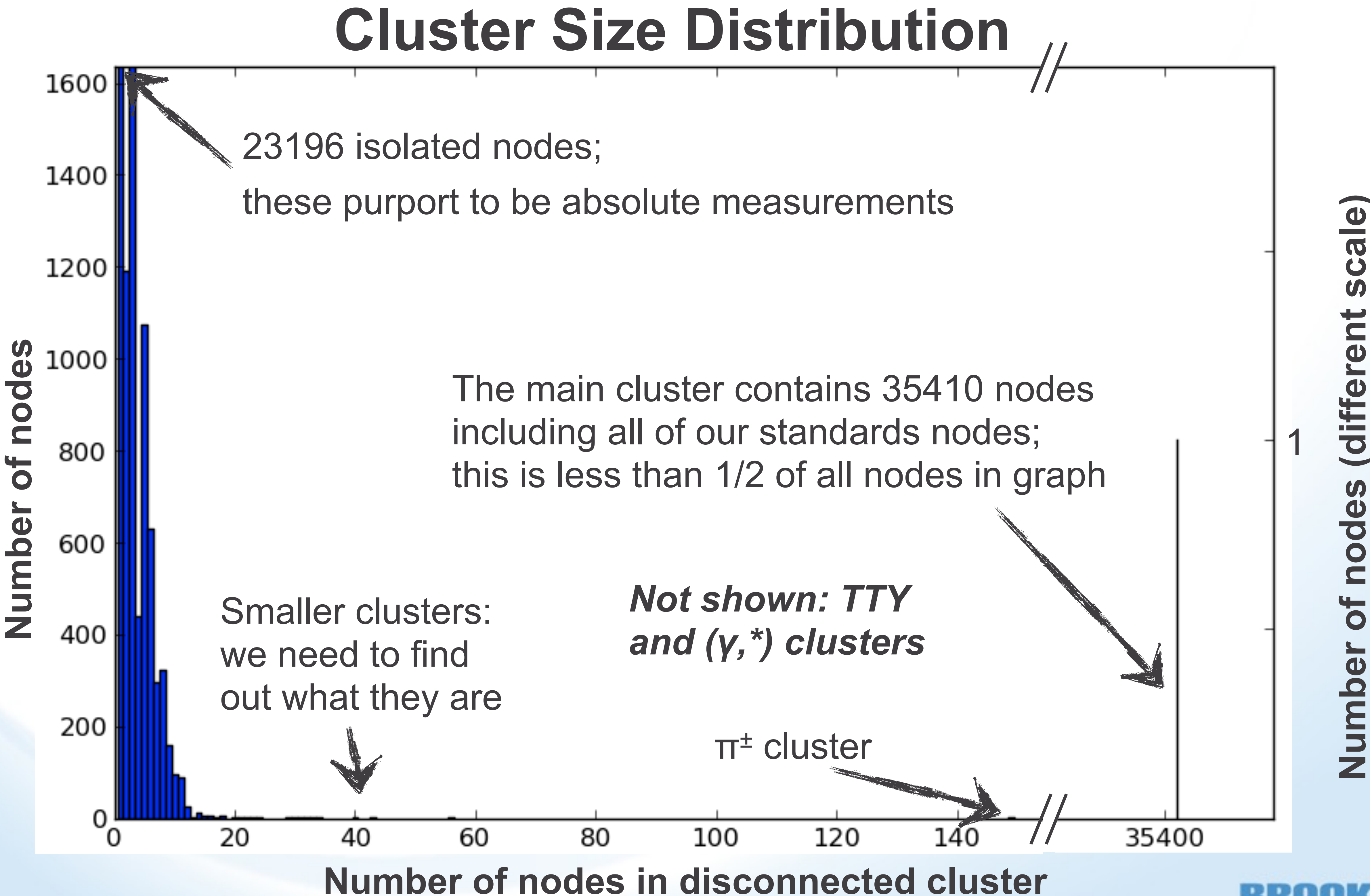
The network
(a closeup of the photonuclear cluster)

nodes: 87925
edges: 276852



Thursday, November 7, 13

The graph is not fully connected;
probability any 2 nodes connected is 7.162e-05



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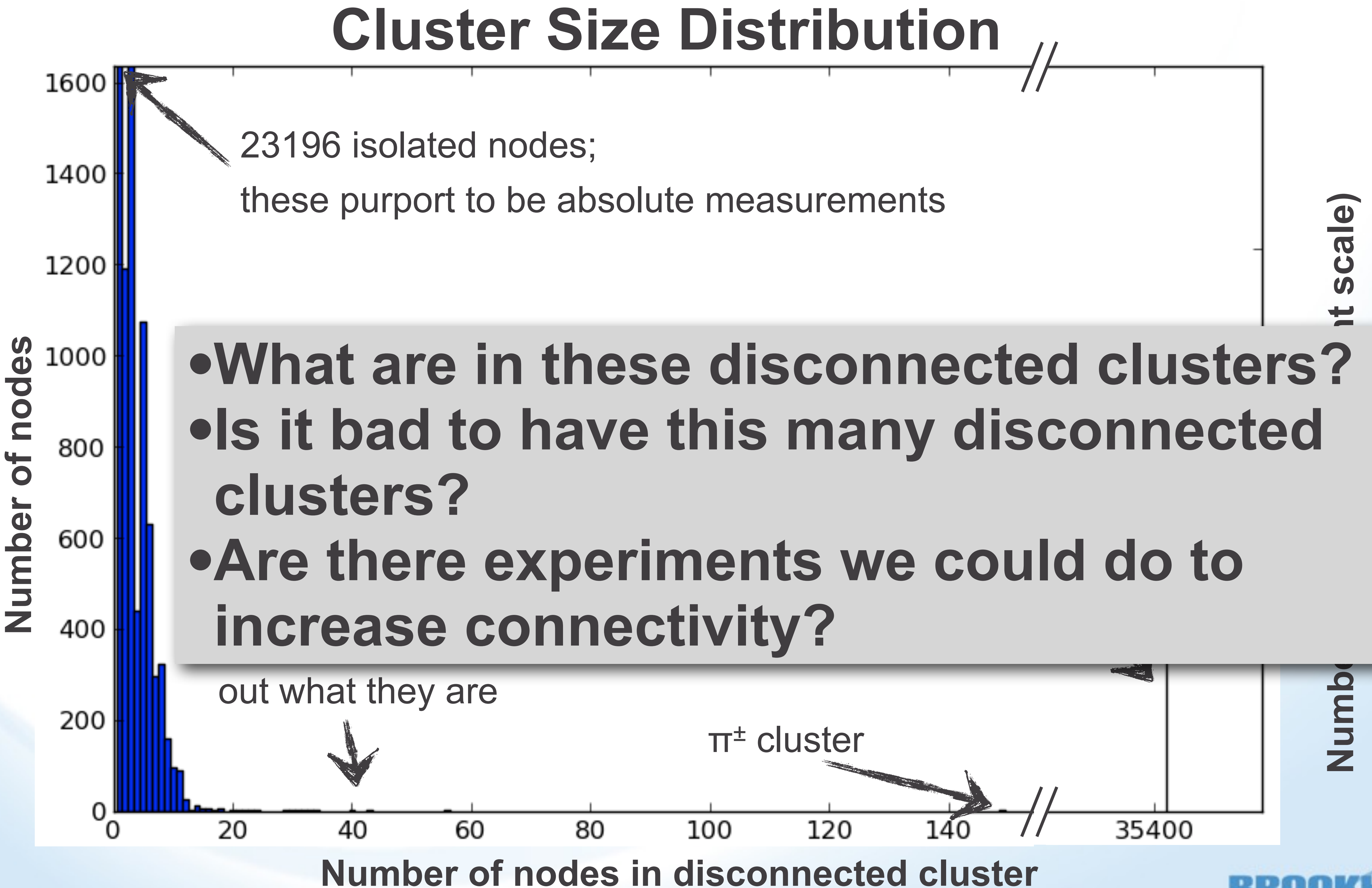

- **What are in these disconnected clusters?**
- **Is it bad to have this many disconnected clusters?**
- **Are there experiments we could do to increase connectivity?**

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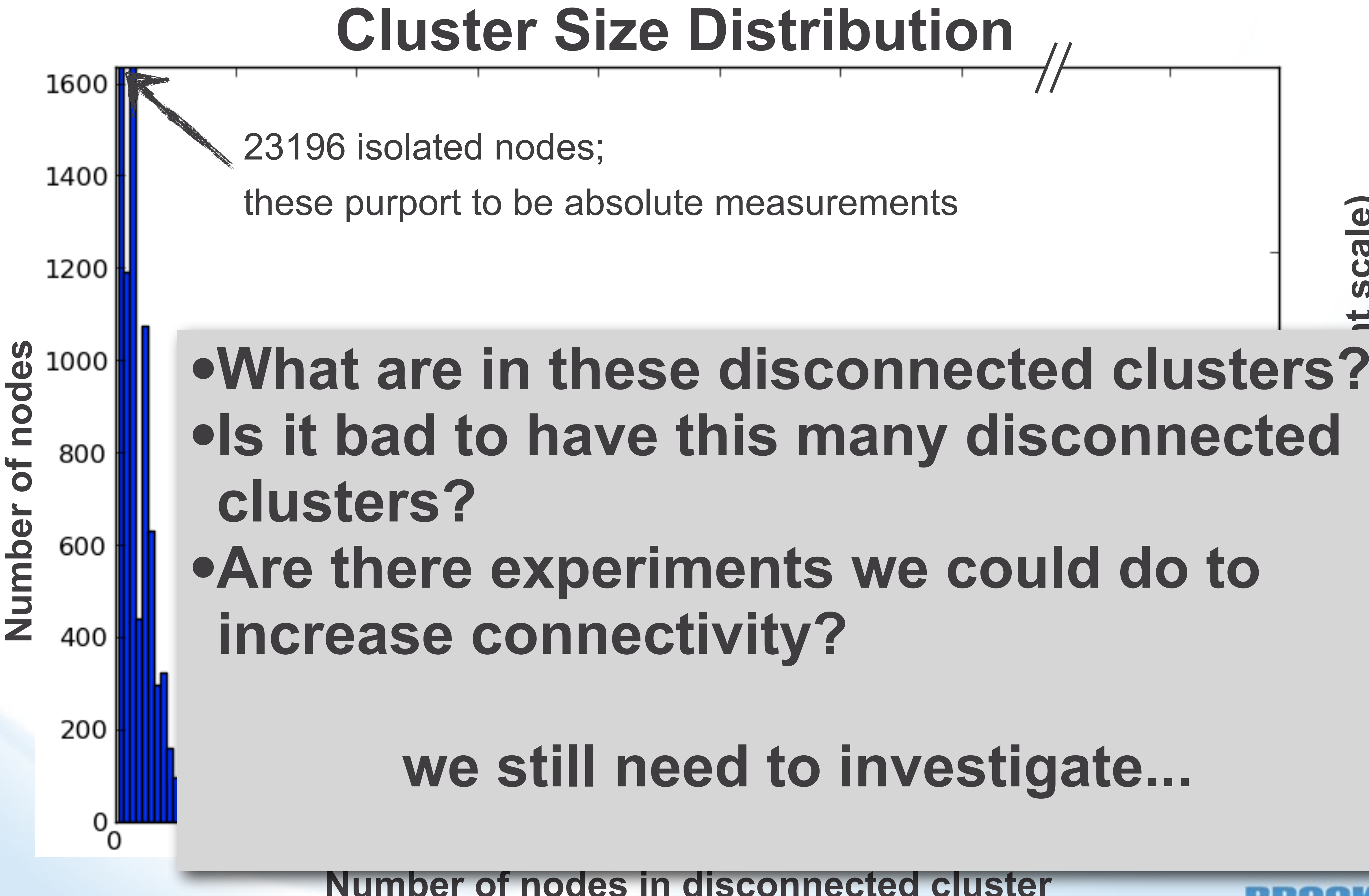
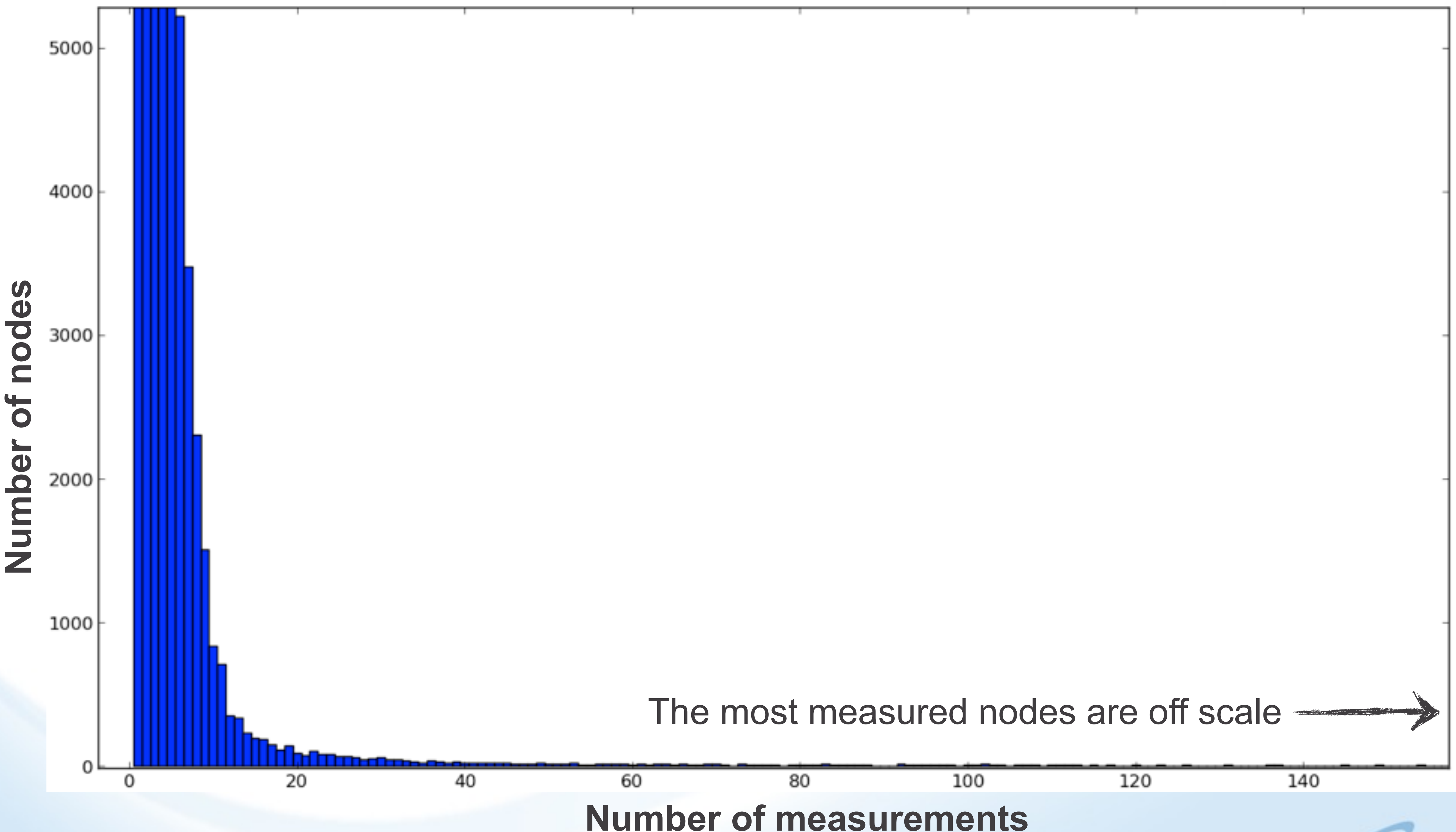


- What are in these disconnected clusters?
- Is it bad to have this many disconnected clusters?
- Are there experiments we could do to increase connectivity?

we still need to investigate...

What is most measured?
These are what experimenters view as important.

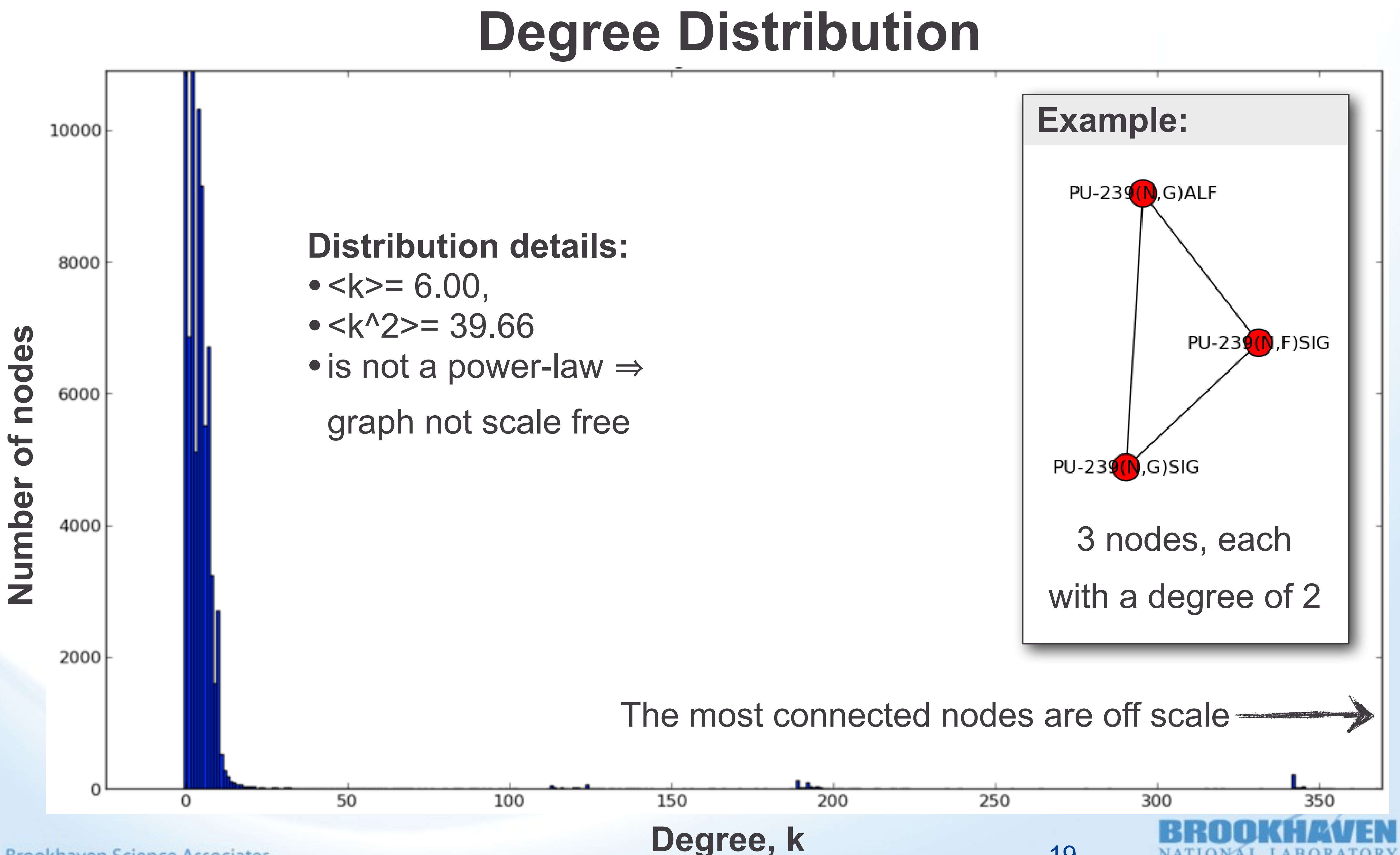


What is most measured?

These are what experimenters view as important.

Node	# Measurements	Degree	Note
27Al(n, α): σ	**5049**	**1281**	
197Au(n, γ): σ	4106	1073	ENDF/Atlas Neutron Standard
27Al(p, X+22Na): σ	3806	2276	IAEA Charged-particle Monitor
235U(n, f): σ	3707	774	ENDF Neutron Standard/CIELO
27Al(p, X+24Na): σ	3626	2122	IAEA Charged-particle Monitor
1H(n, el): σ	2903	1207	ENDF Neutron Standard/CIELO
1H(n, el): dσ/dΩ	2601	953	ENDF Neutron Standard/CIELO
93Nb(n, 2n)92mNb: σ	**2465**	**710**	
27Al(p, n+3p): σ	**2316**	**1535**	
56Fe(n, p)56Mn: σ	2272	833	CIELO
197Au(n, γ): RI	1961	440	ENDF/Atlas Neutron Standard
27Al(n, p)27Mg: σ	**1902**	**544**	
natCu(p, X+65Zn): σ	1899	627	IAEA Charged-particle Monitor
59Co(n, γ): RI	1582	410	Atlas Neutron Standard
58Ni(n, p): σ	**1477**	**344**	
238U(n, f): σ	1394	511	ENDF Neutron Standard/CIELO
59Co(n, γ): σ	1332	578	Atlas Neutron Standard
115In(n, inel): σ	**1161**	**235**	
natMo(p, X+96Tc): σ	**1109**	**600**	
27Al(12C, X+24Na): σ	**1060**	**610**	

The degree of a node is the number of other nodes connected to it



Distribution details:

- <k>= 6.00,
- <k^2>= 39.66
- is not a power-law ⇒ graph not scale free

Most important, by degree

Node	# Measurements	Degree	Note
27Al(p, X+22Na): σ	3806	2276	IAEA Charged-particle Monitor
27Al(p, X+24Na): σ	3626	2122	IAEA Charged-particle Monitor
27Al(p, n+3p): σ	**2316**	**1535**	
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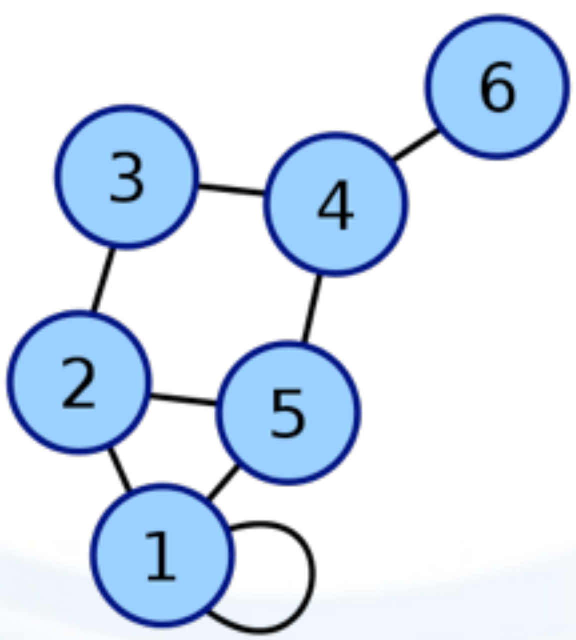
235U(n, f): σ	3707	774	ENDF Neutron Standard/CIELO
93Nb(n, 2n)92mNb: σ	**2465**	**710**	
natCu(p, X+65Zn): σ	1899	627	IAEA Charged-particle Monitor
27Al(12C, X+24Na): σ	**1060**	**610**	
natMo(p, X+96Tc): σ	**1109**	**600**	
natMo(p, X+97Ru): σ	**547**	**594**	
59Co(n, γ): σ	1332	578	Atlas Neutron Standard
27Al(n, p)27Mg: σ	**1902**	**544**	
238U(n, f): σ	1394	511	ENDF Neutron Standard/CIELO
27Al(d, X+24Na): σ	990	507	IAEA Charged-particle Monitor
197Au(n, γ): RI	1961	440	ENDF/Atlas Neutron Standard
10B(n, α): σ	860	432	ENDF Neutron Standard

Other measures of importance

- **Other measures:**
  - Eigenvalue centrality
  - Flow centrality
  - Betweenness
  - ...
- **Rely on adjacency matrix: the matrix of connections between nodes**



$$\begin{pmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Other measures of importance

All require complicated linear algebra on adjacency matrix so behave badly for large graphs

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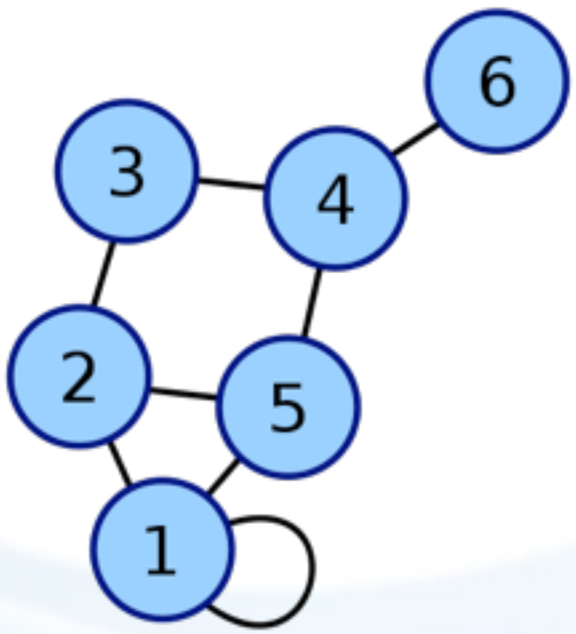

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Testing on subgraphs suggest our graph does not map to a random matrix

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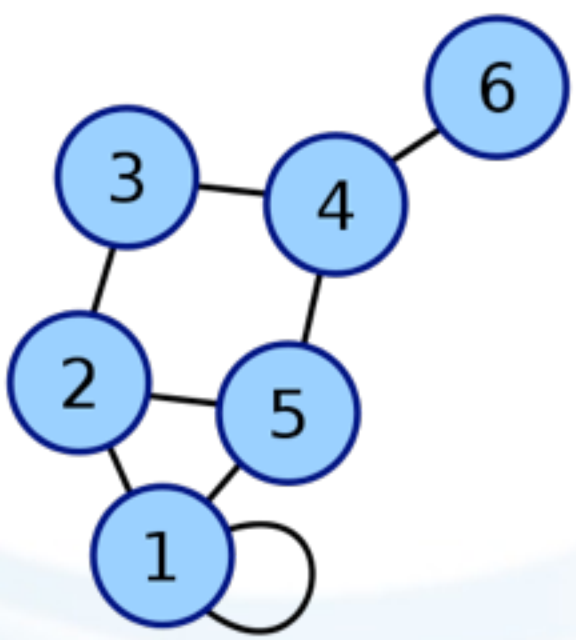

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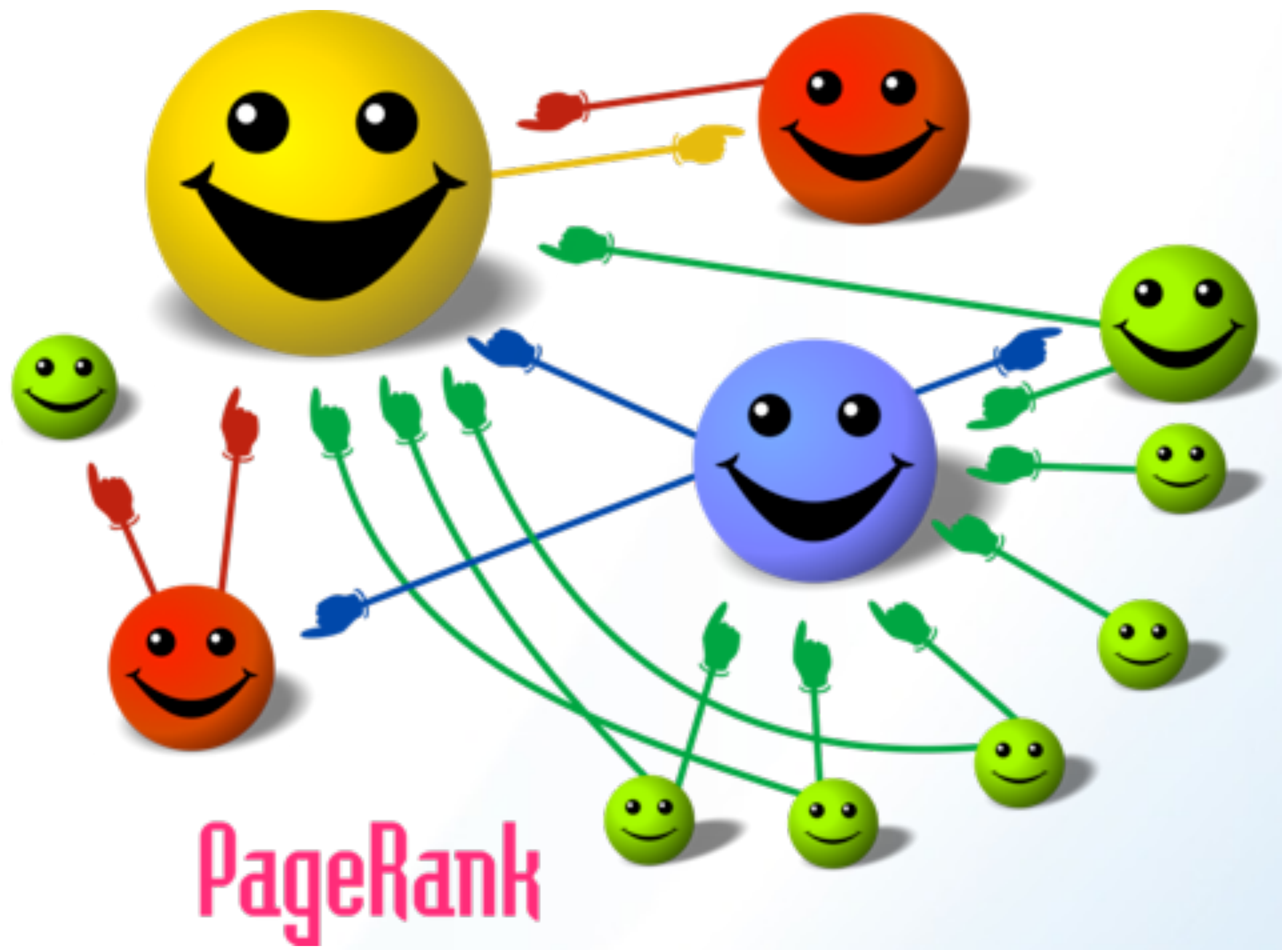
Google PageRank

- **Developed by Larry Page and Sergey Brin**
- **Google's "secret weapon"**
- **Iterative process determines probability to connect to a node**
- **Algorithm**:
  - All nodes start with PR(A)=1
  - Sum PR of all nodes connected to A: PR(A)=PR(B)+PR(C)+PR(D)+...
  - Normalize by PR of all nodes to make into a probability
  - Iterate until convergence



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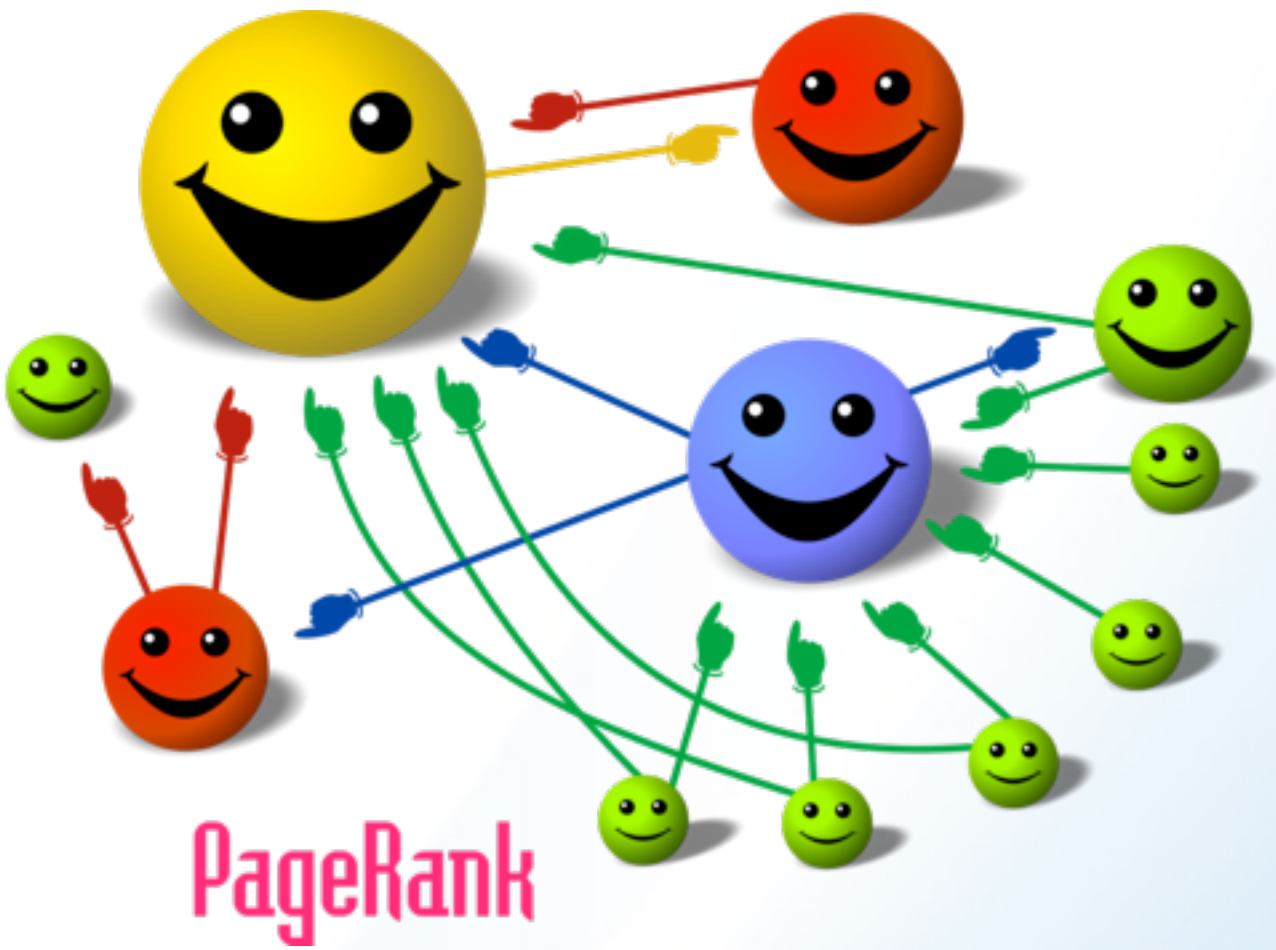

Robust: doesn't need linear algebra that gets flakey with large graphs

Most important by PageRank

Node	# Meas.	PageRank	Note
27Al(p, X+22Na): σ	3806	0.00614361883184	IAEA Charged-particle Monitor
27Al(p, X+24Na): σ	3626	0.00589970042155	IAEA Charged-particle Monitor
27Al(p, n+3p): σ	**2316**	**0.00462137473353**	
1H(n, el): σ	2903	0.00205056586495	ENDF Neutron Standard/CIELO
27Al(n, α): σ	**5049**	**0.0020053191131**	
27Al(12C, X+24Na): σ	**1060**	**0.00198377702452**	
1H(n, el): dσ/dΩ	2601	0.00166716109304	ENDF Neutron Standard/CIELO
197Au(n, γ): σ	4106	0.00161174920126	ENDF/Atlas Neutron Standard
natMo(p, X+96Tc): σ	**1109**	**0.00151848784518**	
natMo(p, X+97Ru): σ	**547**	**0.00150681290335**	
natCu(p, X+65Zn): σ	1899	0.00139242891398	IAEA Charged-particle Monitor
27Al(d, X+24Na): σ	990	0.00125807852791	IAEA Charged-particle Monitor
56Fe(n, p)56Mn: σ	2272	0.00111172026737	CIELO
93Nb(n, 2n)92mNb: σ	**2465**	**0.00104560418528**	
65Cu(p, n): σ	**514**	**0.000851363612779**	
59Co(n, γ): σ	1332	0.000825522215299	Atlas Neutron Standard
natCu(p, X+62Zn): σ	985	0.000815833146368	IAEA Charged-particle Monitor
27Al(n, p)27Mg: σ	**1902**	**0.000759255422463**	
27Al(p, 3n+3p): σ	**528**	**0.000730486791991**	
natTi(p, X+48V): σ	731	0.000711817973821	IAEA Charged-particle Monitor

Recommendations: need to expand our suite of structural materials

- ***Aluminum:* cheap, monoisotopic and easy to work with; the most important structural material next to Iron**
  - n+^{27}Al: (n,α), (n,p)
  - p+^{27}Al: (n,n+3p), ^{22}Na and ^{24}Na production
  - ^{12}C+^{27}Al: ^{24}Na production
- ***Molybdinum* and *Niobium* also very important structural materials:**
  - n+^{93}Nb: ^{93}Nb(n,2n)^{92m}Nb
  - p+^{nat}Mo: ^{96}Tc and ^{97}Ru production
- **Other important structural materials:**
  - n+^{58}Ni: (n,p)
  - n+^{115}In: (n,inel)

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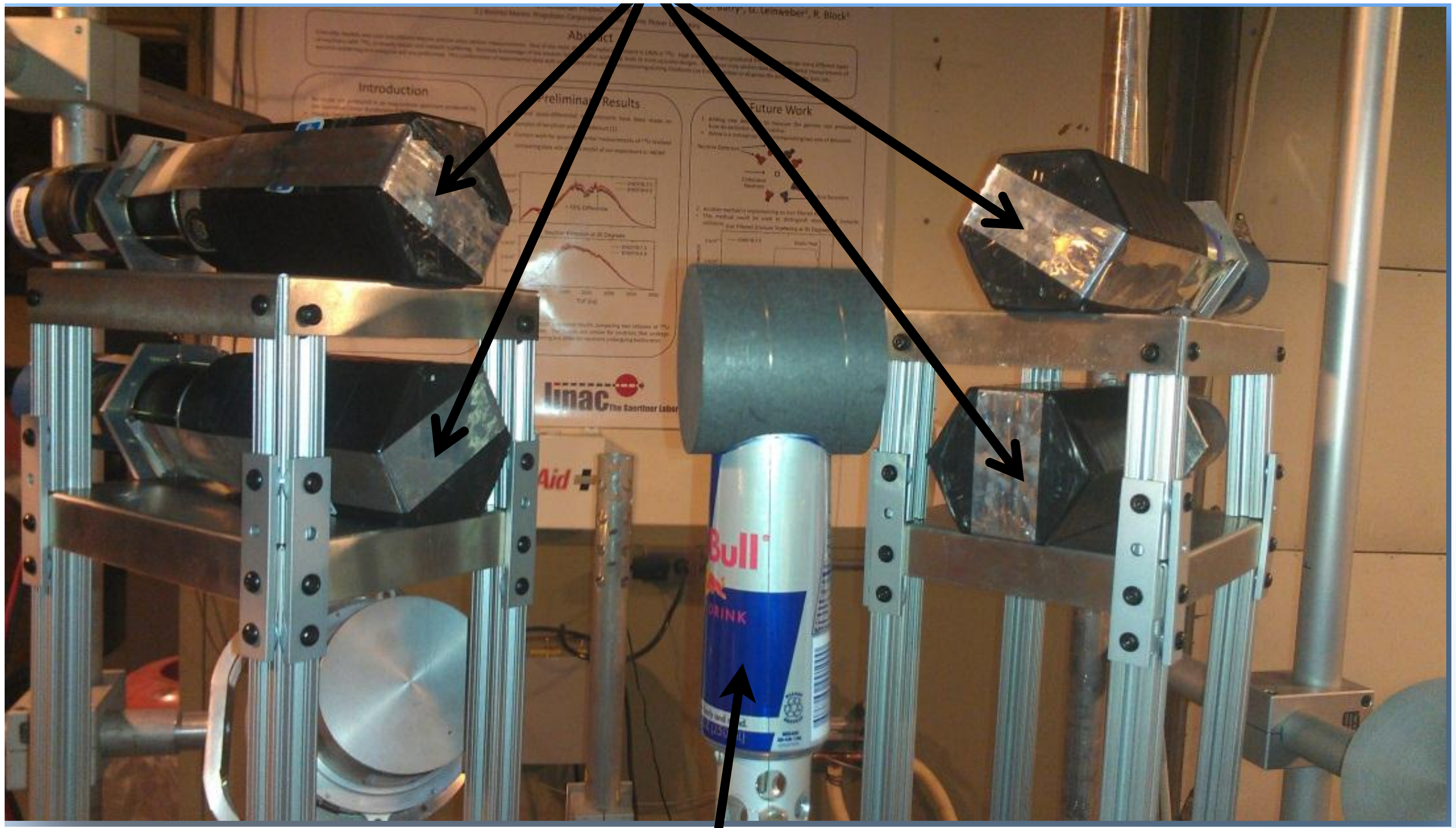
- ***Aluminum:*** **cheap, monoisotopic and easy to work with; the most important structural material next to Iron**
  - n+^{27}Al: (n,α), (n,p)
  - p+^{27}Al: (n,n+3p), ^{22}Na and ^{24}Na production
  - ^{12}C+^{27}Al: ^{24}Na production ← **Yes, ^{12}C as a projectile!**
- ***Molybdinum*** **and** ***Niobium*** **also very important structural materials:**
  - n+^{93}Nb: ^{93}Nb(n,2n)^{92m}Nb
  - p+^{nat}Mo: ^{96}Tc and ^{97}Ru production
- **Other important structural materials:**
  - n+^{58}Ni: (n,p)
  - n+^{115}In: (n,inel)

Aluminum is a very important material for us too

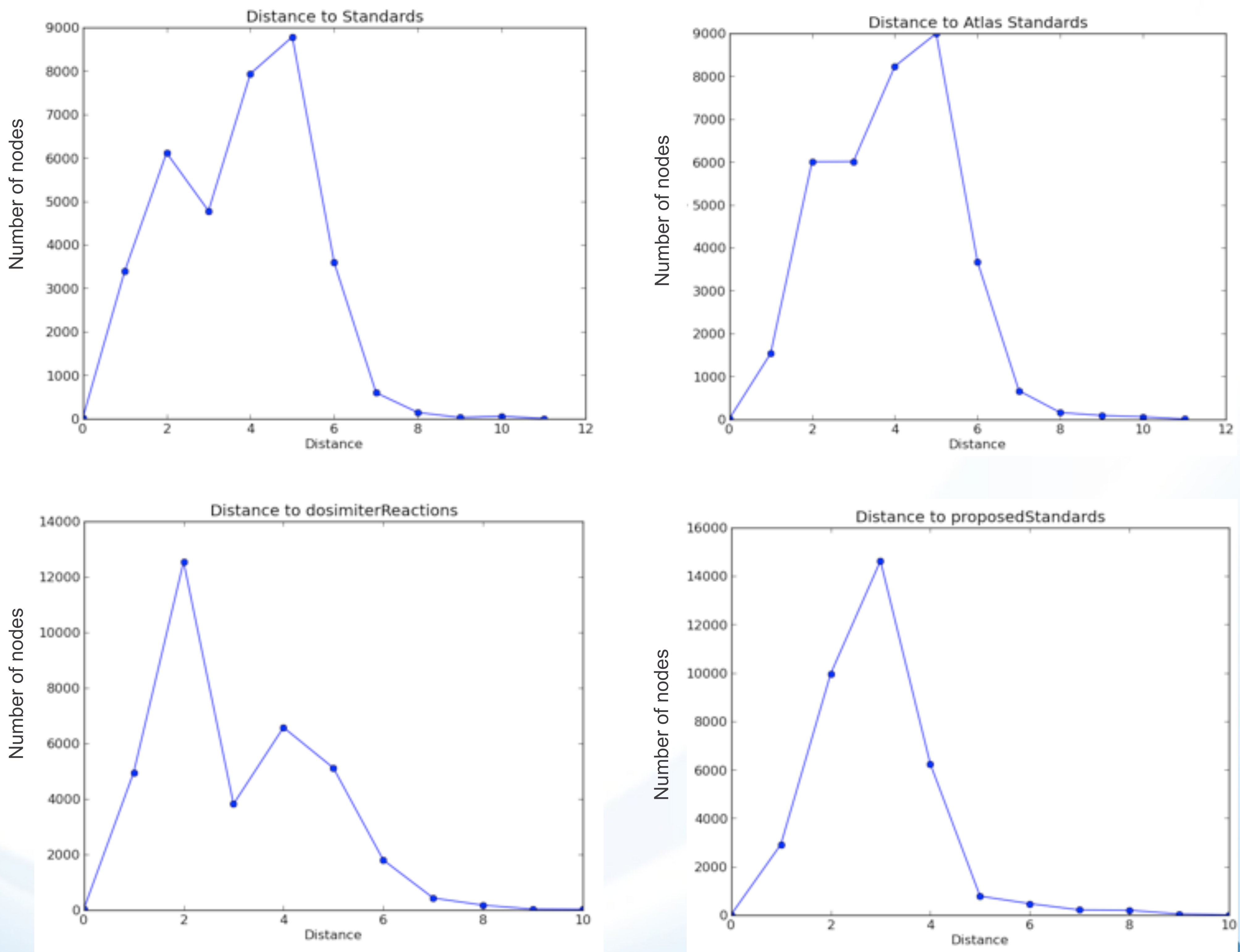
RPI's BaF_2 detector array



From Yaron Danon

RPI's "Low mass sample holder"

Naively, everything should be connected to a monitor of some sort



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