Methods for systematic study of nuclear structure in high-energy collisions

Or: changing nuclei by shifting nucleons

Matthew Luzum

References:
ML, Mauricio Hippert, Jean-Yves Ollitrault; Eur.Phys.J.A 59 (2023) 5, 110; arXiv:2302.14026
João Paulo Picchetti, ML; work in progress
Code available at `https://gitlab.com/mhippert/isobar-sampler`

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Motivation

- Structure of nucleus affects all subsequent processes — important for high-energy collisions
- Ultrarelativistic collisions probe nuclei in a complementary way to low-energy experiments — interesting for low-energy physicists
- Systematic study requires changing nuclear parameters and studying how observables change
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- $\Longrightarrow$ Huge statistics required?
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1. Choose sets of parameter values
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3. Perform collisions and compare observable values

Better procedure

1. Generate discrete nuclear configurations once.
2. For each desired parameter set, modify configurations to obey new distribution by making small shifts to nucleon positions

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Outline

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Aside: Step + Gauss distribution

- Nice alternative to approximate a Woods-Saxon
- Not necessary, but has nice properties and makes some things easier

- Nucleon position is sum of two random vectors sampled from:
  1. 3D step $P_s(\mathbf{x}) \sim \Theta(R_s - r)$
  2. 3D Gaussian $P_g(\mathbf{x}) \sim e^{-\frac{r^2}{2w^2}}$
- Rough rule of thumb:

$$R_s(R, a) \simeq R\left[1 + 1.5\left(\frac{a}{R}\right)^{1.8}\right]$$

$$w(R, a) \simeq 1.83\, a$$

$$\rho_c(\mathbf{x}) = \int P_s(\mathbf{z}) P_g(\mathbf{x} - \mathbf{z}) d^3 z$$

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$$\rho_c(\mathbf{x}) \sim \left[\frac{\sqrt{2}w}{r}\left(e^{-\frac{(r+R_s)^2}{2w^2}} - e^{-\frac{(r-R_s)^2}{2w^2}}\right) + \sqrt{\pi}\left\{\mathrm{Erf}\left(\frac{r+R_s}{\sqrt{2}w}\right) - \mathrm{Erf}\left(\frac{r-R_s}{\sqrt{2}w}\right)\right\}\right]$$

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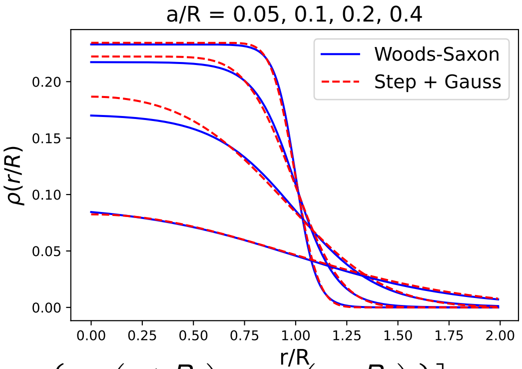

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Step+Gauss distribution advantages

Benefits of Step+Gauss

- Can directly modify Woods-Saxon parameters (R, a) without the following numerical methods
- Fast/easy to sample
- Nice analytic properties — smooth at origin
- Trivial relation between point nucleon density and charge density

Outline

Changing nuclear shape

- 1-body nucleon distribution parameterized as

$$\rho(r) \propto \frac{1}{1 + e^{\frac{r-R}{a}}}$$

$$\tilde{\rho}(r,\theta,\phi) \propto \frac{1}{1 + e^{\frac{r-R-R\sum \beta_{\ell,m} Y_{\ell,m}}{a}}} = \rho(r - R\sum_{\ell,m} \beta_{\ell,m} Y_{\ell,m})$$

- Define continuous parameter t that takes you from spherical ($t = 0$) to desired deformed distribution ($t = 1$)

$$\tilde{\rho}(\vec{x}, t) \equiv \rho(r - t\sum_{\ell,m} R\beta_{\ell,m} Y_{\ell,m})$$

- Idea: change nuclear properties by shifting the position of nucleons

$$\implies \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

- Start with uncorrelated nucleons satisfying $\rho(r)$, end with uncorrelated nucleons satisfying $\rho(r - R\sum_{\ell,m} \beta_{\ell,m} Y_{\ell,m})$

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- One nice solution (at $t = 0$):

$$\vec{v} = \nabla \Phi(\vec{x})$$

$$\Phi = \sum R\beta_{\ell,m} f_{\ell,m}(r) Y_{\ell,m}$$

$$0 = f''_{\ell,m} + f'_{\ell,m}\left(\frac{2}{r} + \frac{\rho'}{\rho}\right) - \frac{\ell(\ell+1)}{r^2} f_{\ell,m} - \frac{\rho'}{\rho}$$

$$0 = f_{\ell,m}(r \to 0)$$

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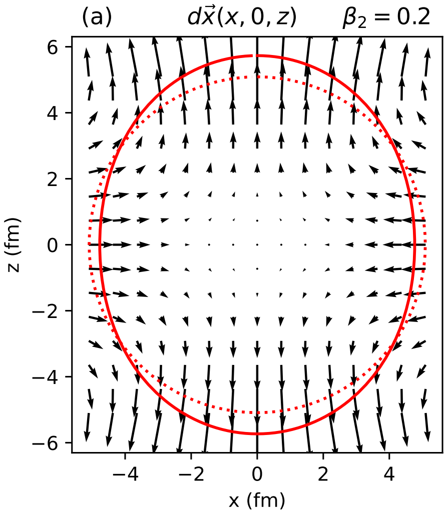

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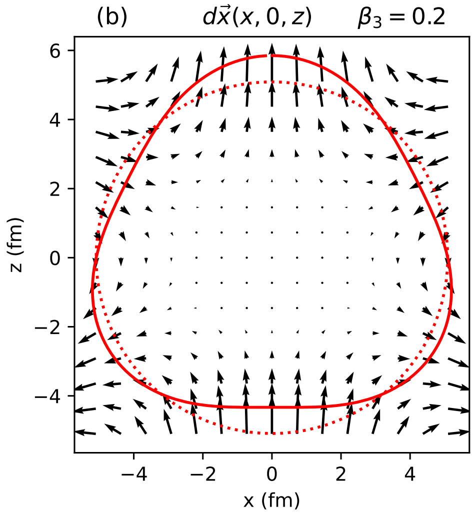
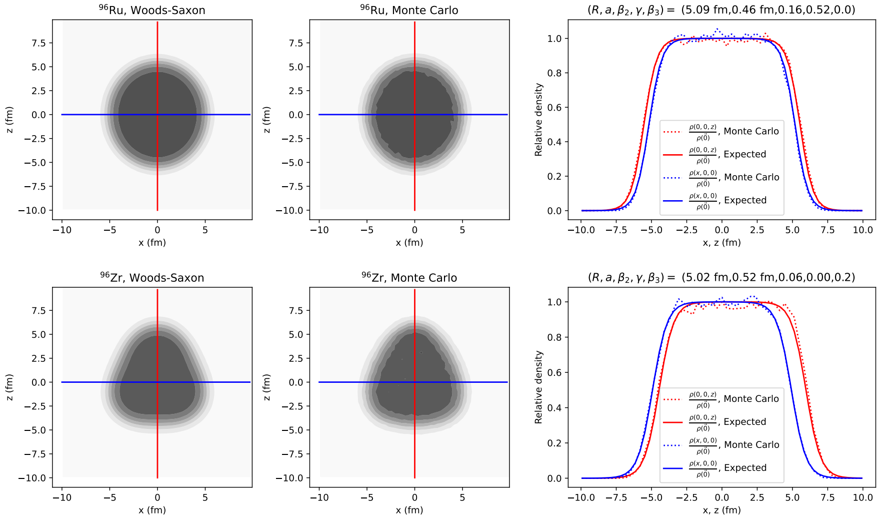


Numerical results (100k nuclei)

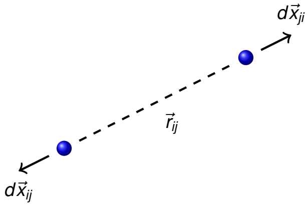


Outline

- Short-range interactions cause particles to be correlated

$$\rho_2(\vec{x}_1, \vec{x}_2) = \rho(\vec{x}_1)\rho(\vec{x}_2)\left[1 + C(\vec{r}_{12})\right]$$

- Idea: induce correlation C from uncorrelated set by shifting particles



$$d\vec{x}_i = \sum_{j \neq i} d\vec{x}_{ij} = \sum_{j \neq i} \frac{1}{2}\left(\tilde{r}_{ij} - r_{ij}\right)\hat{r}_{ij}$$

Finding $dr = \tilde{r} - r$

- Conserve pairs:

$$\int_0^r d^3 r' = \int_0^{\tilde{r}} d^3 r' (1 + C(\vec{r}'))$$

- Invert relation to solve for $\tilde{r}$
- Example:
  $C(r)$ extracted from 10000 ^{96}Ru configurations generated from realistic 2- and 3-body interactions

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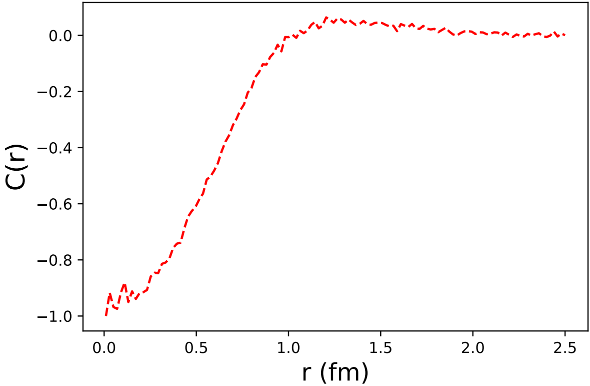

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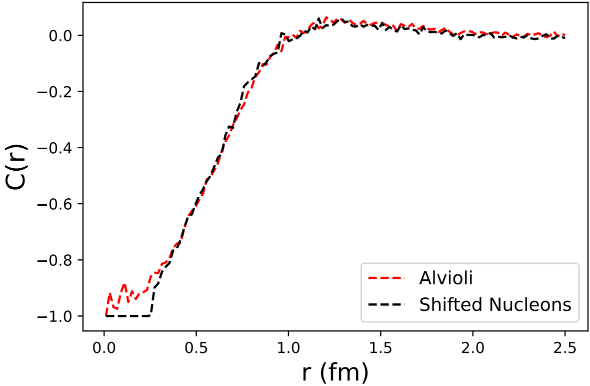

Other benefits

Advantages

Compared to usual implementation (i.e., "exclusion radius"):

- Can study correlation of arbitrary shape
- Compatible with any 1-body distribution (no problems with triaxial nuclei)
- Better control over 2-body and 1-body distributions

Compared to sophisticated Monte-Carlo of Alvioli, Strikman, *et al.*:

- Faster and easier
- Anyone can generate their own configurations
- (But lacks 3-body correlations)

Outline

Benchmarks

How much benefit can you get?

- Simple benchmark test: Trento model at $b = 0$.
- Ratio of eccentricities $\varepsilon_n\{k\}$ with realistic correlation / no correlation
- Saves $\sim$3 orders of magnitude in computing resources!

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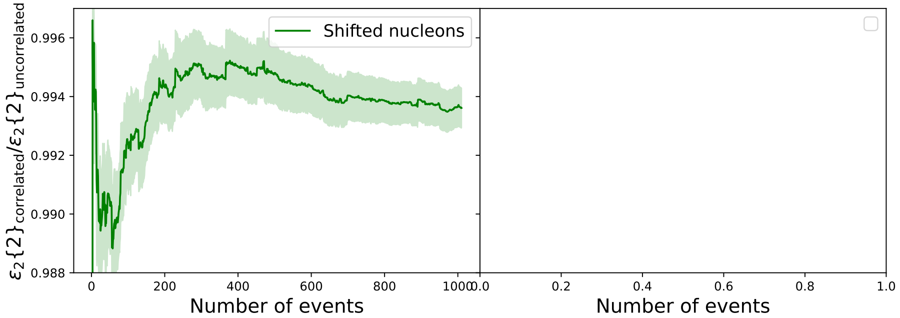

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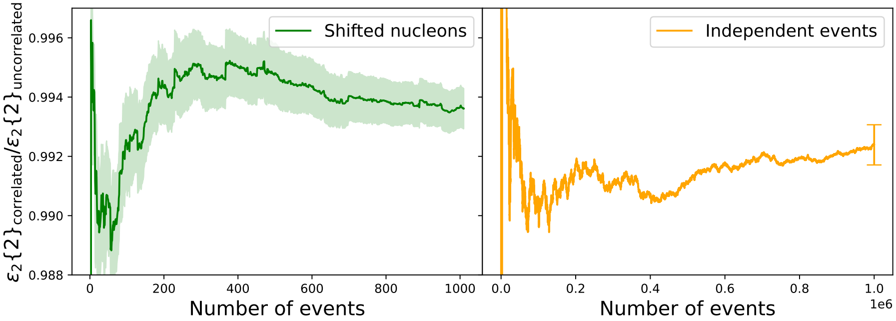

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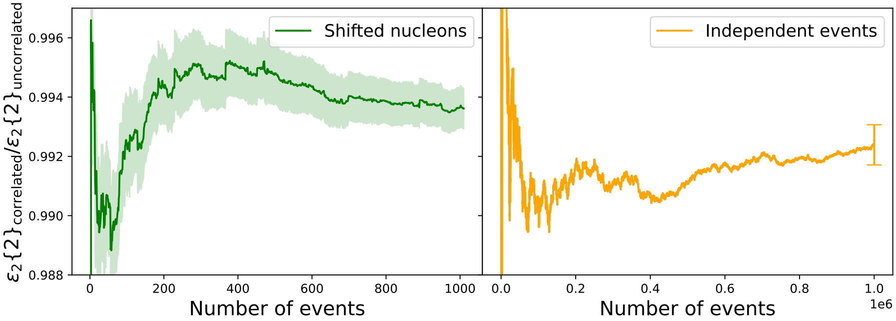

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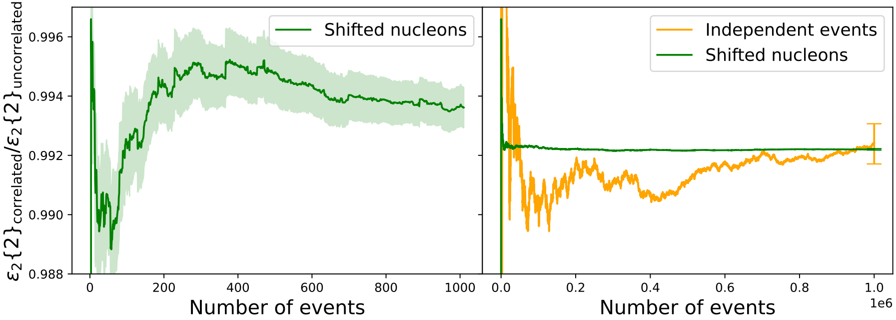

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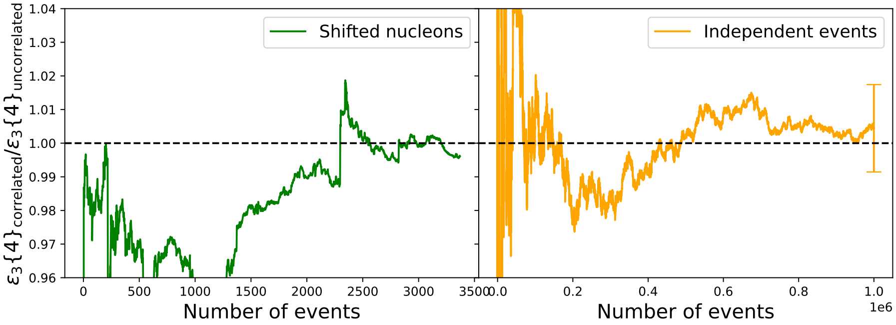

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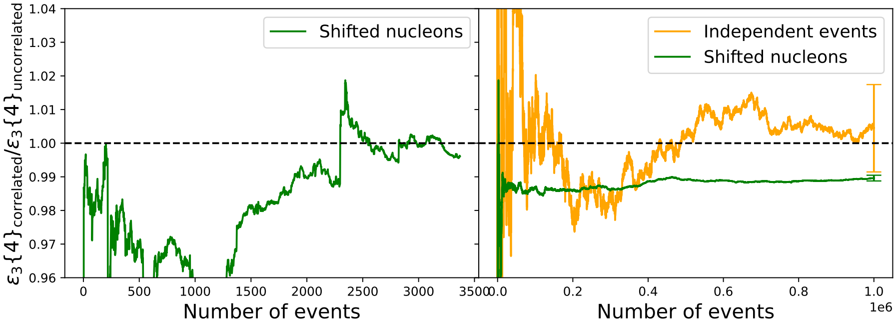

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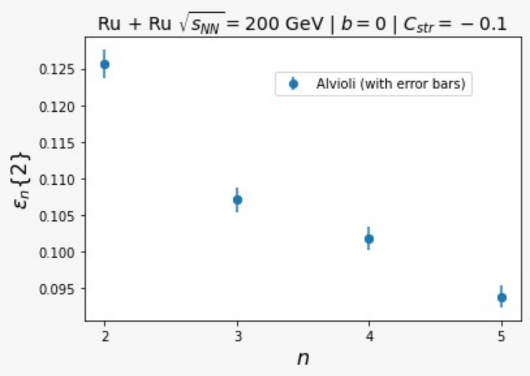
- Illustration:
  Use Alvioli nuclei in Trento collisions — ε_n as (pseudo-)data
- Most common implementation: exclusion distance
- Is this a reasonable approximation? If so, what's the most realistic exclusion radius?



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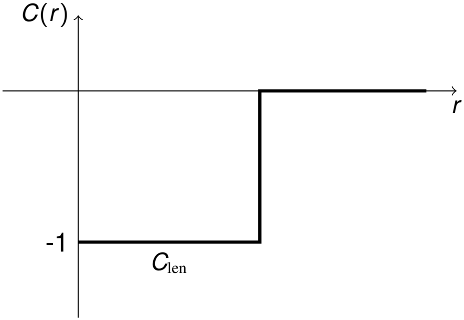

Bayesian estimation of exclusion radius

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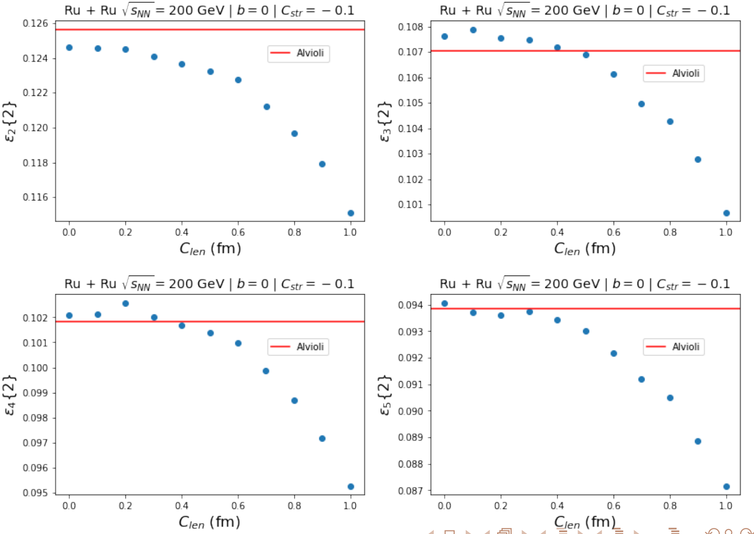
- Uncorrelated nucleons no worse than finite exclusion.
- Better to allow for more general parameterizations — easily done with these methods (using publicly available code)



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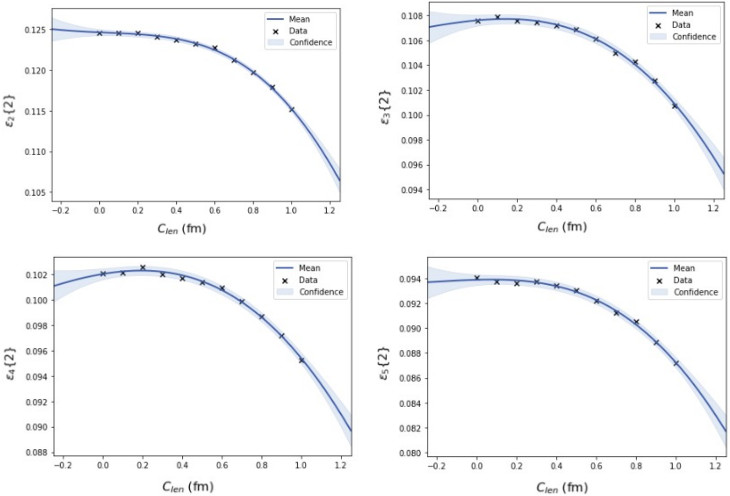

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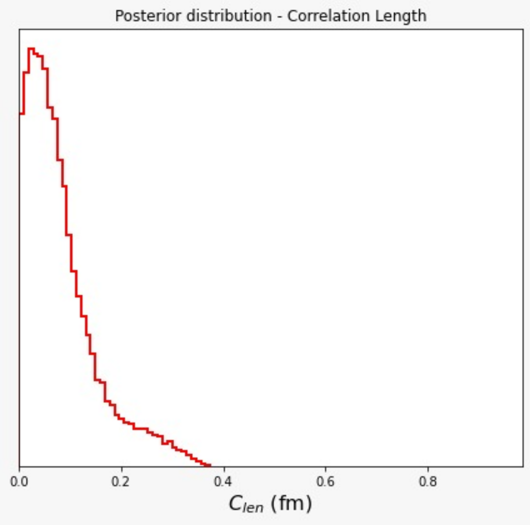

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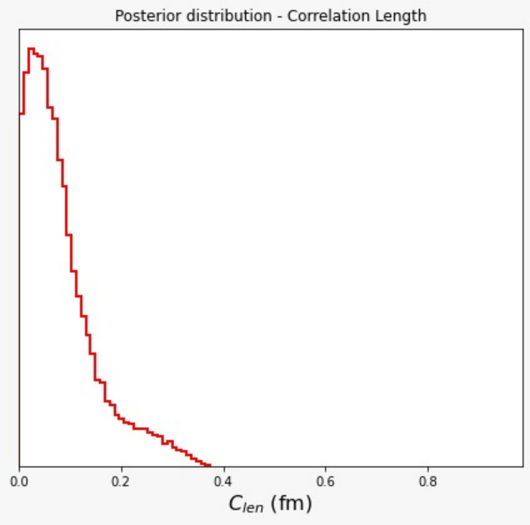


Summary

- Statistical demands significantly reduced by correlating statistical fluctuations — change nuclear properties by shifting nucleons
- Opens many opportunities for systematic study of nuclear structure
- Can study arbitrary shape parameters (R, a, $\{\beta_{\ell,m}\}$) and short-range correlation $C(\vec{r})$
- Simple exclusion radius not a good approximation of realistic correlations.
- Python code to generate nuclei available at `https://gitlab.com/mhippert/isobar-sampler`
    - *Warning:*
      Must synchronize other fluctuations in collision — impact parameter, orientation of nuclei, etc.

Extra Slides

Other benchmarks (participant Glauber model)

Par.	Param. Change	$\varepsilon_2\{2\}$ Change	Improv. Factor	Avg. Shift
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$(0.2\ \mathrm{fm})^3$	0.13%	2900	0.002 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$\times 2$	0.27%	1100	0.005 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$\times 4$	0.53%	350	0.009 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$(0.4\ \mathrm{fm})^3$	1.1%	180	0.017 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$\times 2$	2.0%	98	0.032 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$\times 4$	3.8%	54	0.059 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$(0.8\ \mathrm{fm})^3$	7.3%	25	0.11 fm
$C_{\mathrm{str}} C_{\mathrm{len}}^3$	$\times 2$	14%	13	0.19 fm

Takeaways

- Significant improvement possible
- Main limitation: nucleon shift can change participant $\leftrightarrow$ spectator
- Smaller differences in nuclei $\implies$ larger improvement factor
- Exact numbers will depend on model, centrality, etc.

Other benchmarks (participant Glauber model)

Par.	Param. Change	$\varepsilon_n\{2\}$ Change	Improv. Factor	Avg. Shift
β_2	0.005	0.02%	170	0.008 fm
β_2	0.01	0.10%	100	0.02 fm
β_2	0.02	0.39%	42	0.03 fm
β_2	0.05	2.3%	12	0.08 fm
β_2	0.1	8.8%	4.7	0.17 fm
β_2	0.2	31%	2.1	0.33 fm
β_3	0.01	0.05%	79	0.01 fm
β_3	0.05	1.6%	13	0.06 fm
β_3	0.1	6.3%	5.0	0.12 fm
β_3	0.2	23%	2.2	0.25 fm

Takeaways

- Smaller efficiency gain for angular deformation (for same average shift distance)
- (Particles near edge of nucleus have larger than average shift)

Valid correlation functions

- Note that the number of pairs is fixed:

$$\rho(\vec{x}_1)\rho(\vec{x}_2)\left[1 + C(\vec{r}_{12})\right] = \rho_2(\vec{x}_1, \vec{x}_2)$$
$$\Longrightarrow \int d^3x_1 d^3x_2 \rho(\mathbf{x}_1)\rho(\mathbf{x}_2) C(\vec{r}_{12}) = 0$$

- Respecting sum rule important for maintaining fixed 1-body distribution
- If nominal short-range correlation doesn't satisfy, we add constant

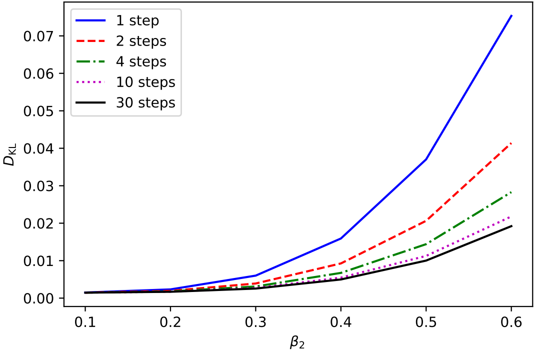
$$C(r) = C_{\text{short}}(r) + C_\infty$$
$$C_\infty \simeq -C_{\text{vol}} \int d^3x \rho(\mathbf{x})^2$$

Quantifying 1-body density

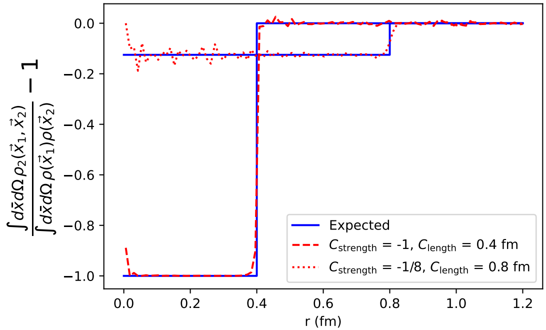
A natural way to compare probability distributions is the Kullback–Leibler (KL) divergence

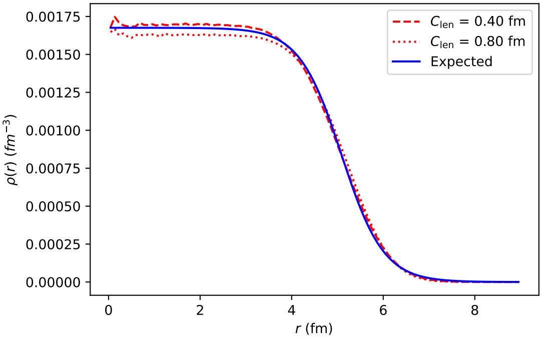
$$D_{\mathrm{KL}}(\rho_1||\rho_2) \equiv \int d^3x\,\rho_1(\mathbf{x}) \log \frac{\rho_1(\mathbf{x})}{\rho_2(\mathbf{x})}.$$

Accuracy increases if the nucleon shift is broken into multiple steps.



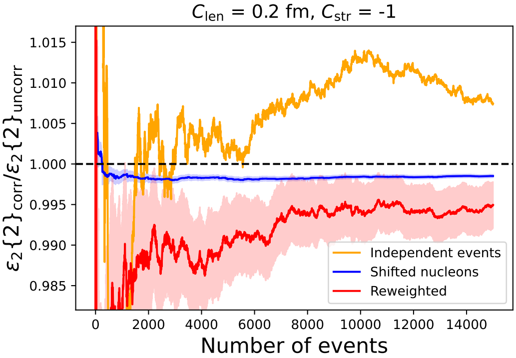
1- AND 2-PARTICLE DENSITIES





Reweighting method

- Can probe different points in parameter space with *no* extra simulations by reweighting the collision events. However, it converges very poorly unless the parameter values are very close.
- It is more efficient than shifting nucleons for small changes ($\Delta\beta \lesssim 0.01$), but loses efficacy quickly for larger changes, becoming worse than independent sampling for $\Delta\beta \gtrsim 0.08$ or $\Delta(C_{\mathrm{str}} C_{\mathrm{len}}^3) \gtrsim (0.3\ \mathrm{fm})^3$ and rapidly degrading beyond that.



FINDING $dr = \tilde{r} - r$

- Conserve pairs:

$$\int_0^r d^3r' = \int_0^{\tilde{r}} d^3r'(1 + C(\vec{r}'))$$

- Invert relation to solve for $\tilde{r}$
- Simple example: step function with variable length $C_{\text{length}} \geq 0$ and strength $C_{\text{strength}} \geq -1$

FINDING $dr = \tilde{r} - r$

- Conserve pairs:

$$(r^3 - \tilde{r}^3) = 3 \int_0^{\tilde{r}} dr' \, r'^2 C(r')$$

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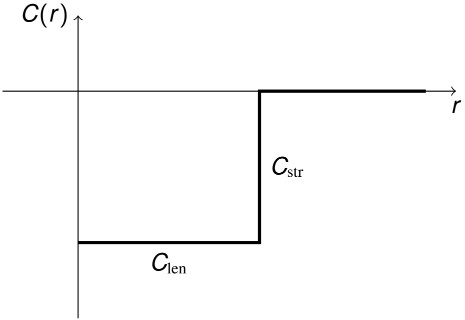

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