Efficient 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://github.com/mluzum/Isobar-Sampler`

University of São Paulo

Exploring nuclear physics across energy scales 2024:
Intersection between nuclear structure and high energy nuclear collisions
April 15–27, 2024

Motivation

- Standard methods to study nuclear structure in high-energy collisions require significant statistics
- Example: short-range correlations
- There is a better way!

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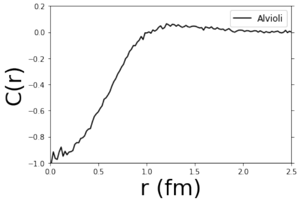

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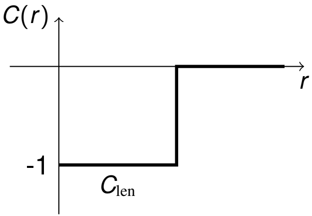

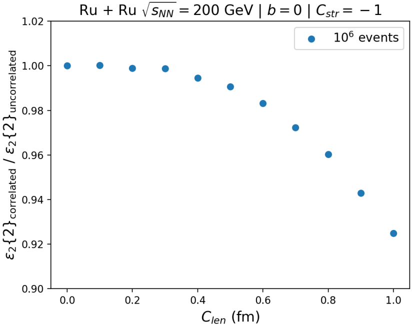

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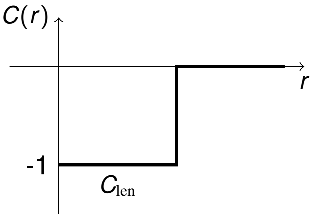

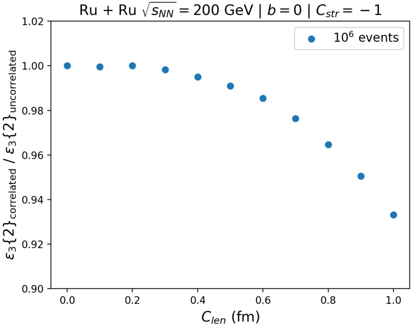

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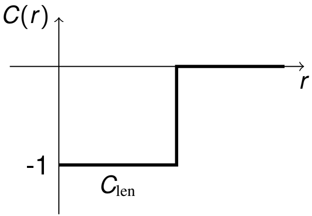

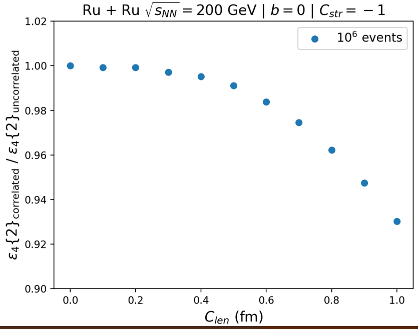

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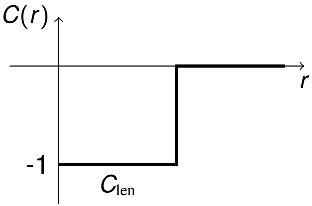

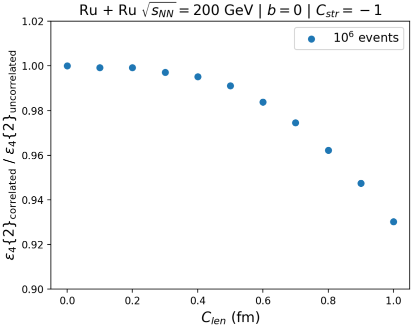

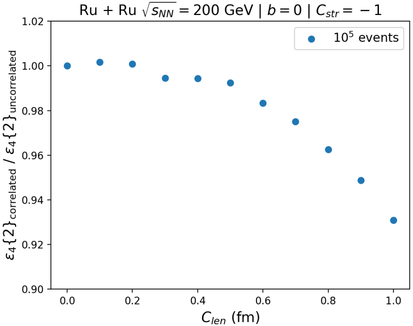

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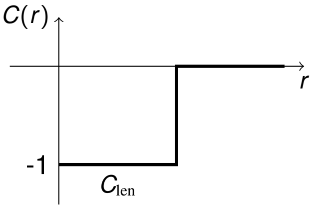

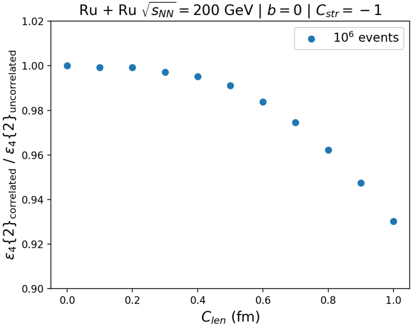

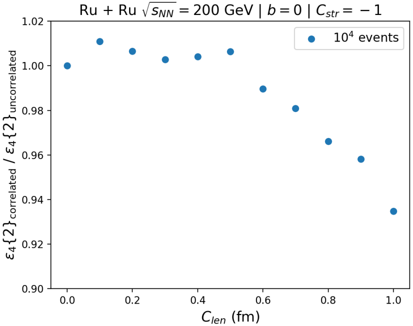

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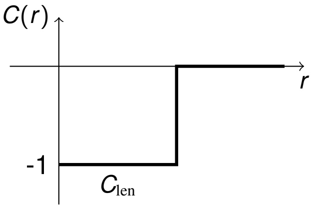

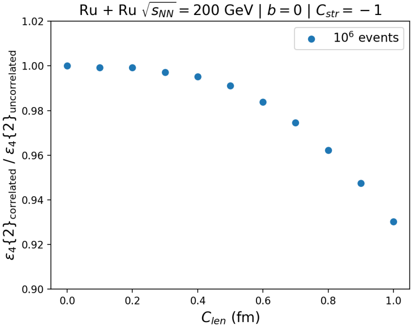

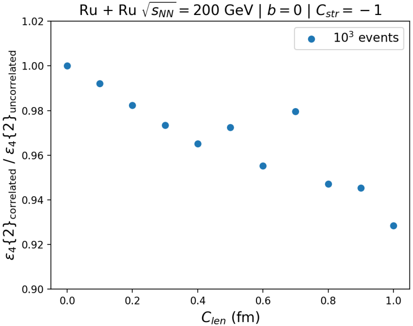

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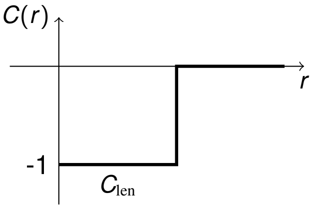

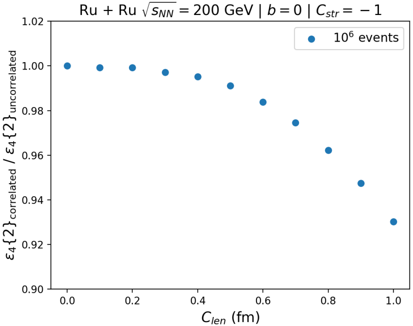

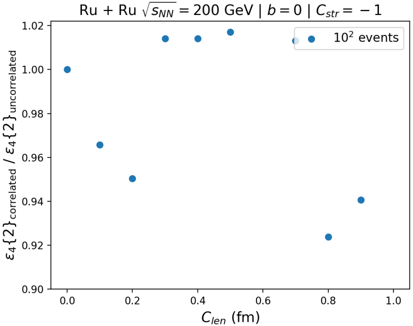

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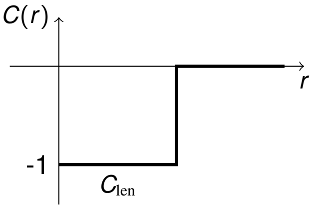

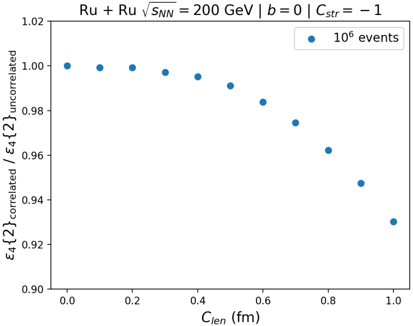

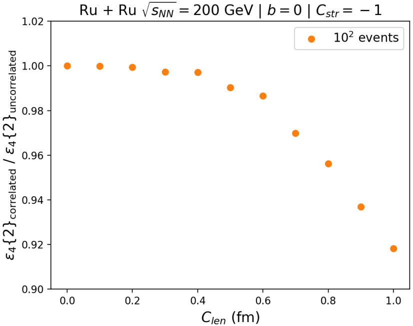

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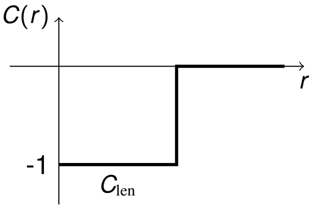

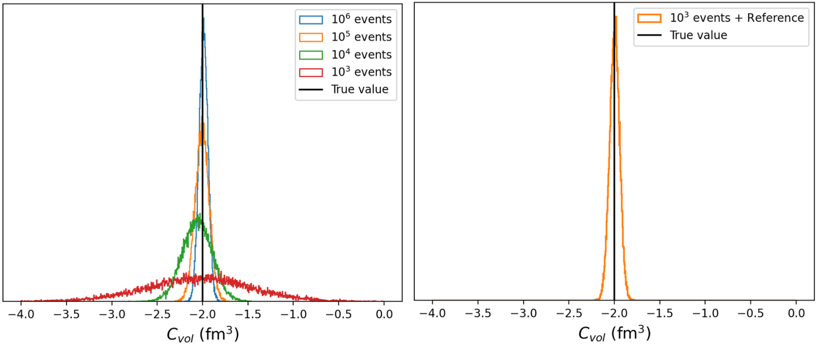

Exploring parameter space

- To isolate parameter dependence, should control fluctuations. E.g.:
  - Does changing particlization increase/decrease yields? $\rightarrow$ Use same freeze-out surface and change only δf
  - Does viscosity increase/decrease elliptic flow? $\rightarrow$ Use same initial conditions when changing η/s
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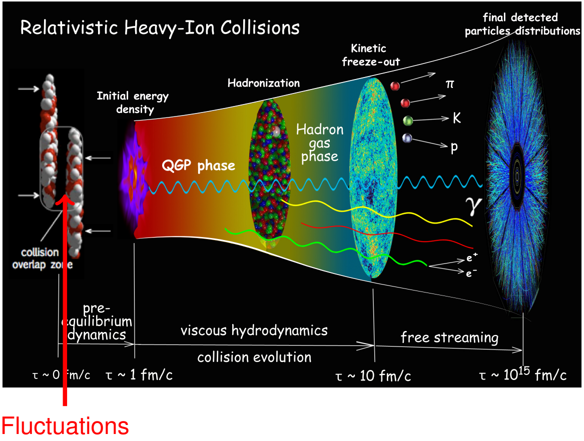

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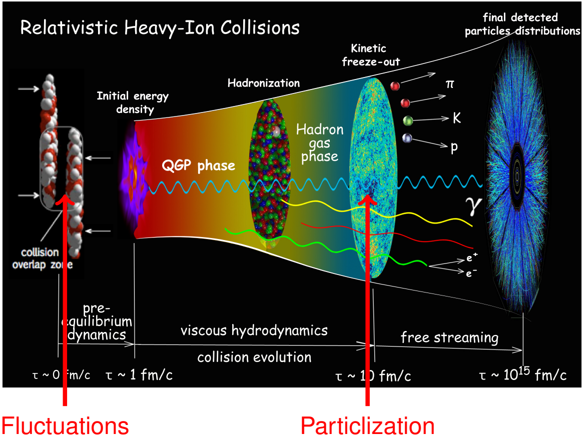

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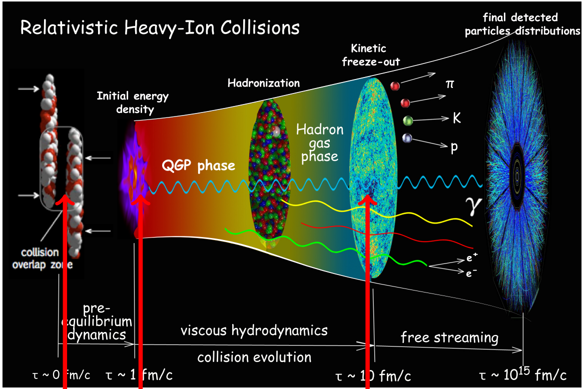

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Initial Scattering

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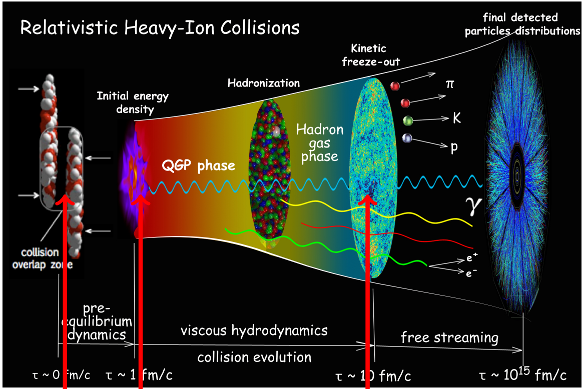

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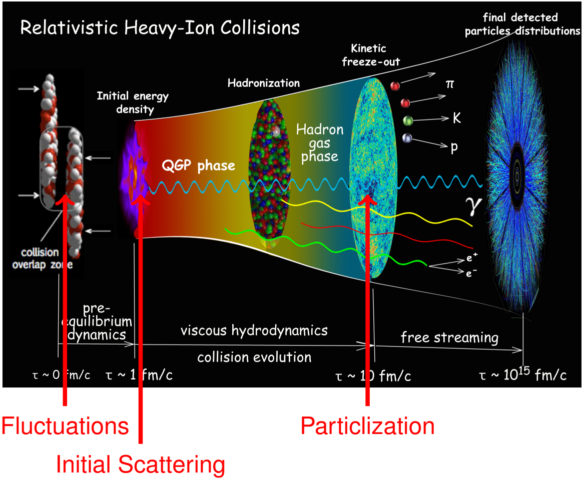
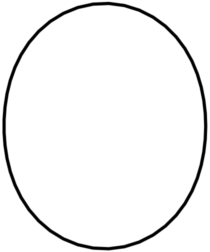
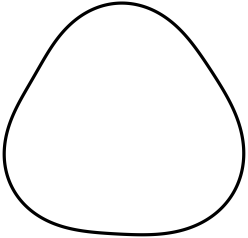


Changing nuclei by shifting nucleons

Procedure used until now

1. Independently generate new nuclear configurations for each parameter set
2. Perform collisions and compare observable values





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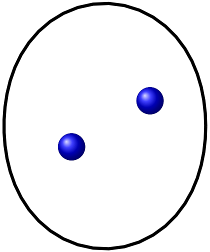

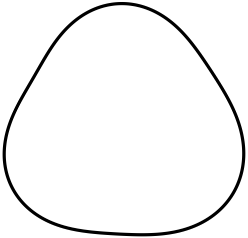

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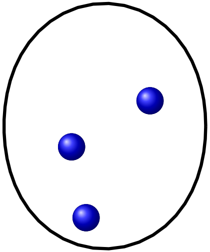

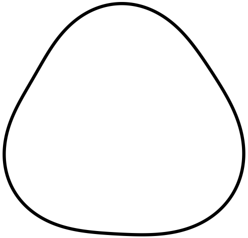

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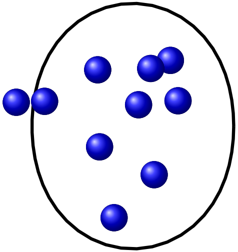

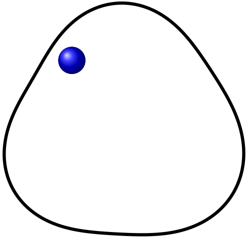

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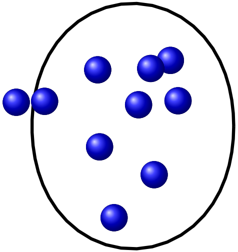

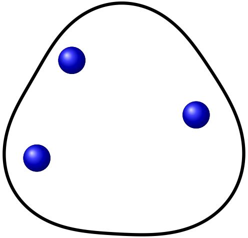

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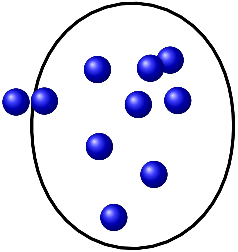

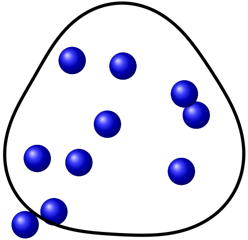

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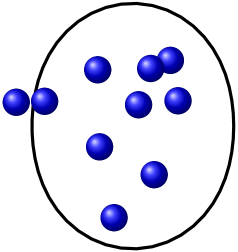
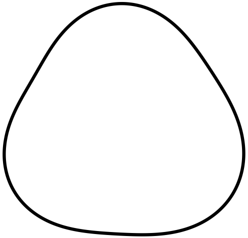
- Sample nucleus once, shift nucleons to change nuclear properties





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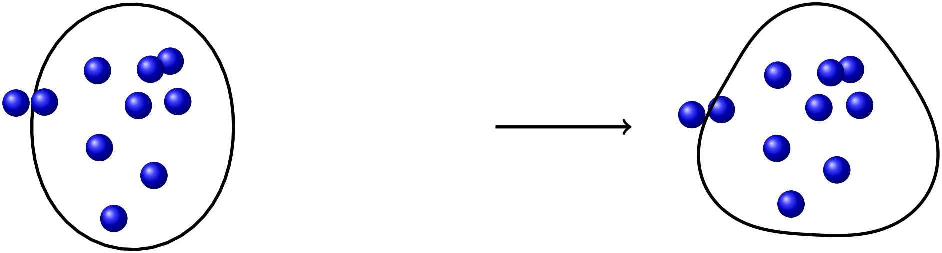

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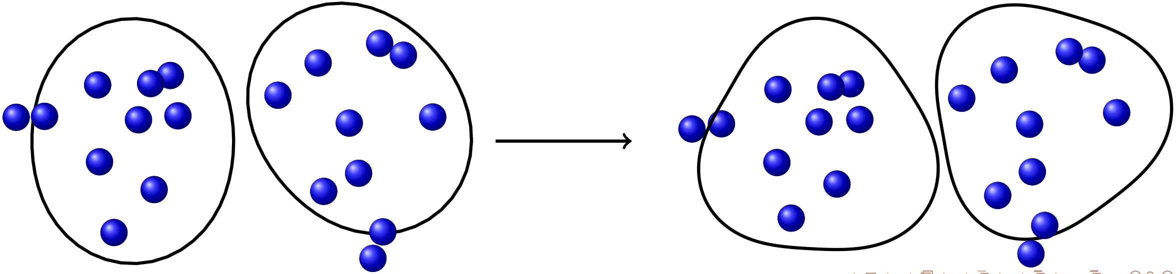

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Aside: Step + Gauss distribution

- 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:

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

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

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

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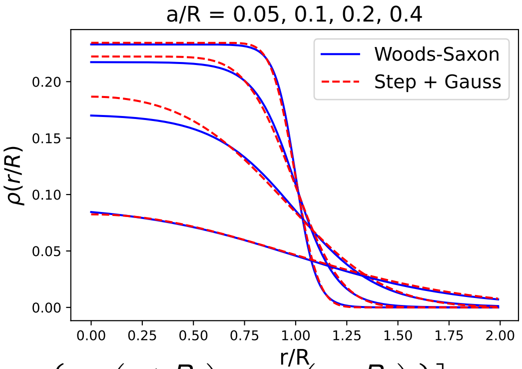

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Step+Gauss distribution advantages

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

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

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

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

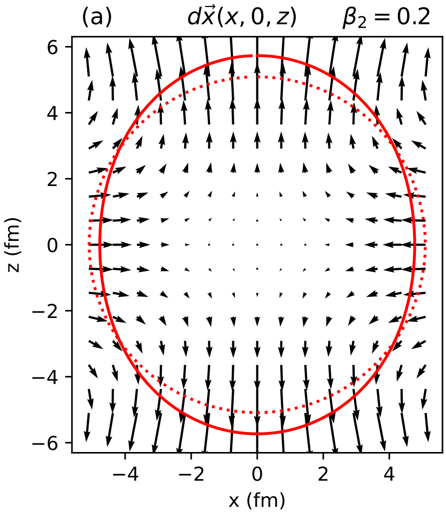
$$\vec{v} = \nabla \Phi(\vec{x})$$

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

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

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

$$1 = f'_{\ell,m}(r \to \infty)$$



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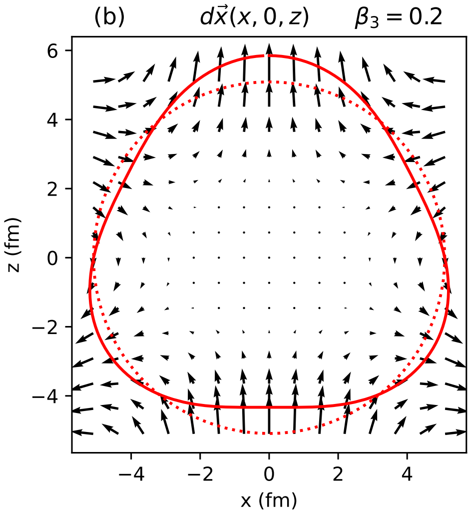
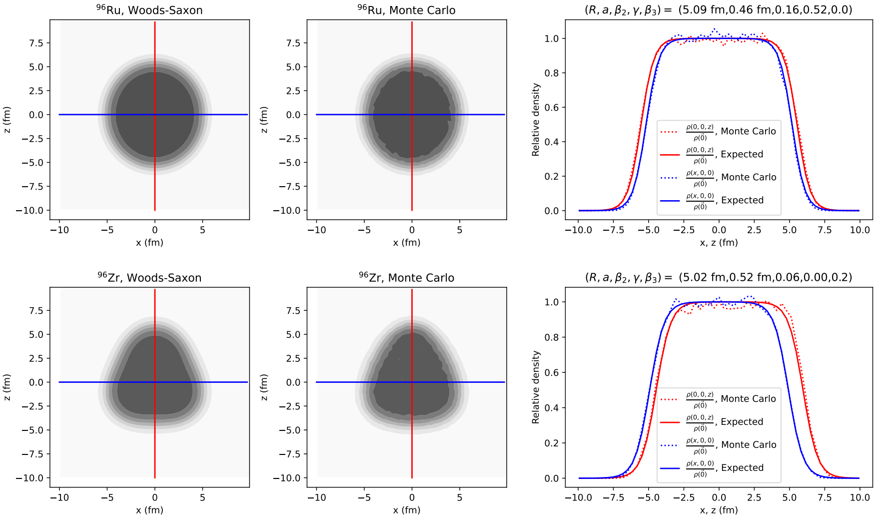


NUMERICAL RESULTS (100K NUCLEI)



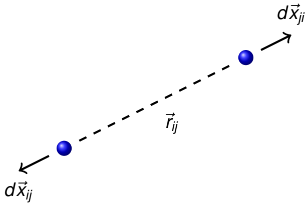
Outline

Short-range correlations

- 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

  Hammelmann, Soto-Ontoso, Alvioli, Elfner, Strikman; Phys. Rev. C 101, 061901(R)

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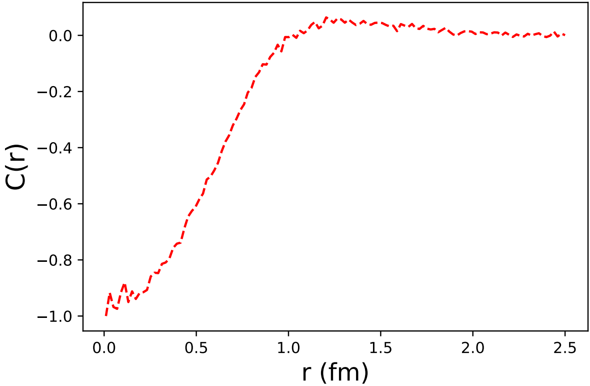

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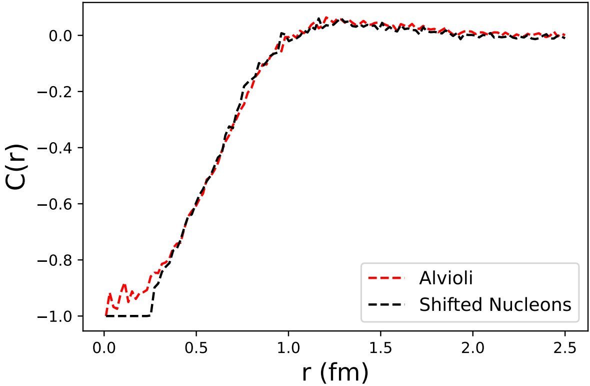

Other benefits

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
- Can save $\sim$3 orders of magnitude in computing resources!

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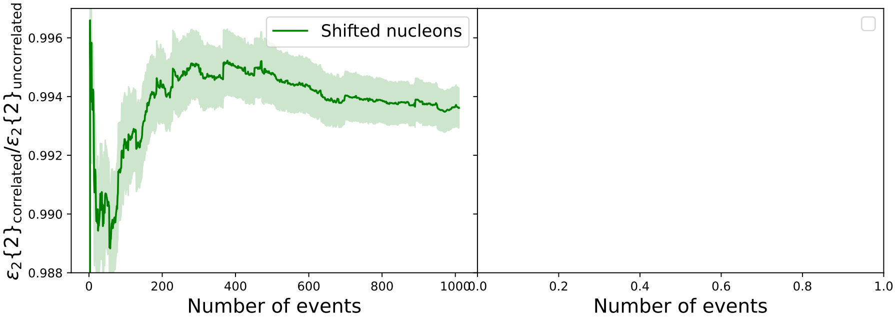

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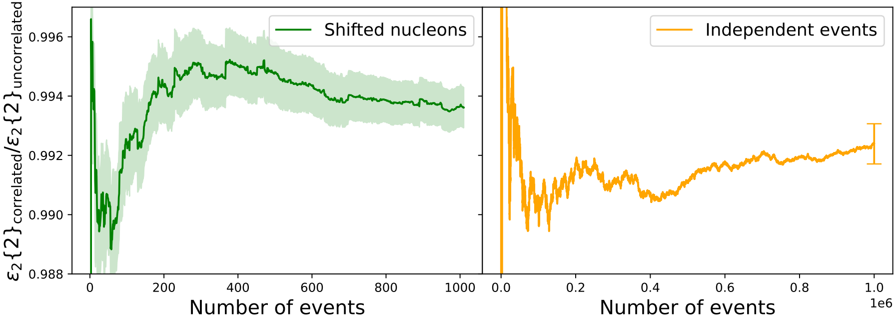
- Can save ~3 orders of magnitude in computing resources!



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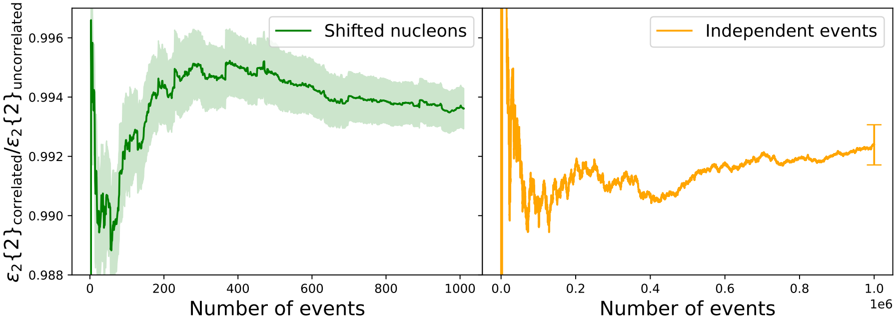

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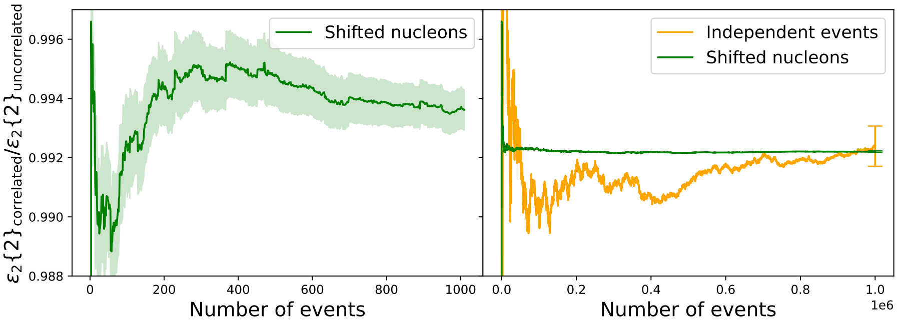

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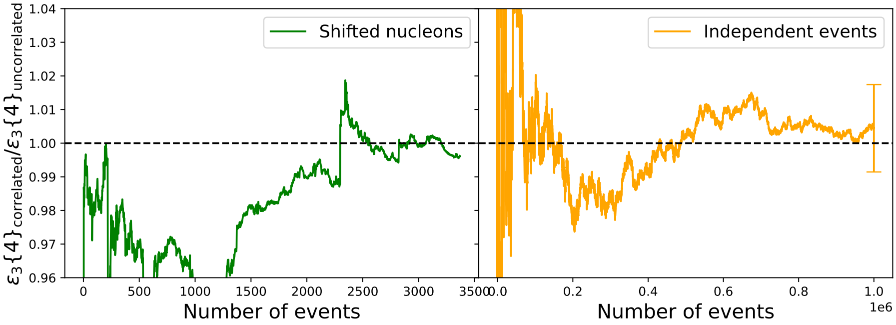

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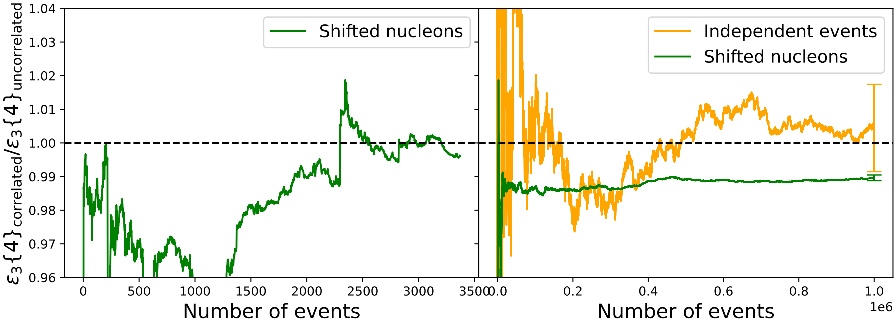
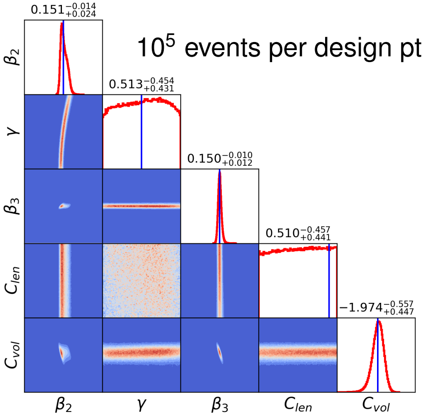
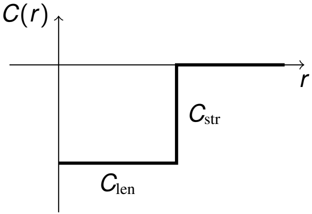


Outline

Bayesian closure test (Preliminary)

- Illustration: Bayesian closure test — infer parameter values from known model output
- Parameters: β_2. γ, β_3, $C_{\rm len}$, $C_{\rm vol} = \int d^3r C(r)$
- Observables at $b = 0$: $\varepsilon_2\{2\}$, $\varepsilon_3\{2\}$, $\varepsilon_4\{2\}$, $\varepsilon_5\{2\}$, $\varepsilon_2\{4\}$, $\frac{dE}{d\eta}$





Parameter	Prior range
β_2	[0,0.3]
γ	[0,1]
β_3	[0,0.3]
$C_{\rm len}$	[0,1] fm
$C_{\rm vol}$	[-4.18,0] fm^3

Parameter	True value
β_2	0.15
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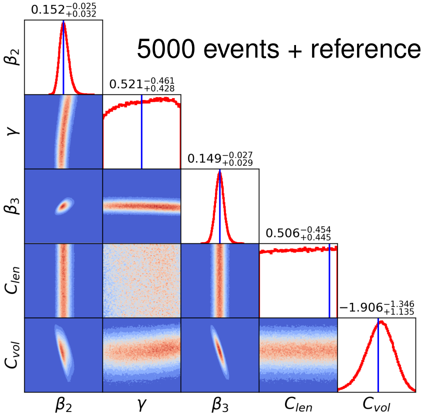

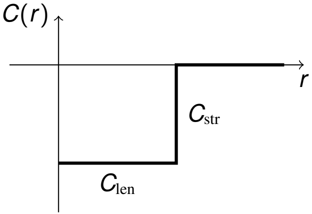

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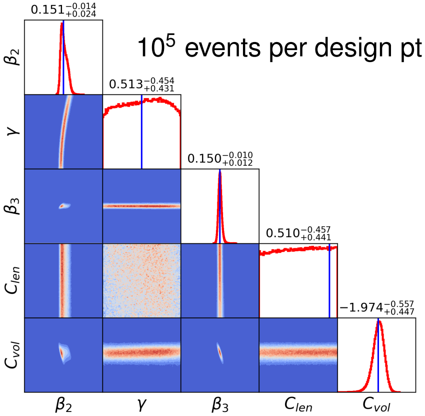
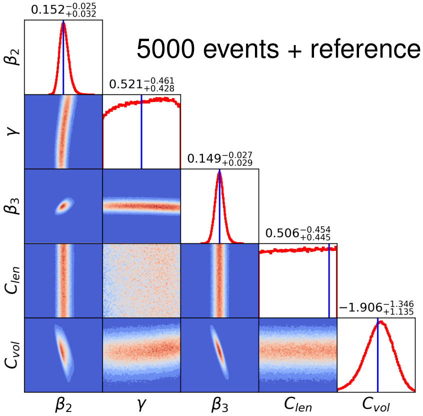




Summary

- Statistical demands significantly reduced by correlating statistical fluctuations — change nuclear properties by shifting nucleons
- Can study arbitrary shape parameters $(R, a, \{\beta_{\ell,m}\})$ and short-range correlation $C(\vec{r})$
- Opens many opportunities for systematic study of nuclear structure
- Python code to generate nuclei available at `https://github.com/mluzum/Isobar-Sampler`

Extra Slides

Other benchmarks (participant Glauber model)

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

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

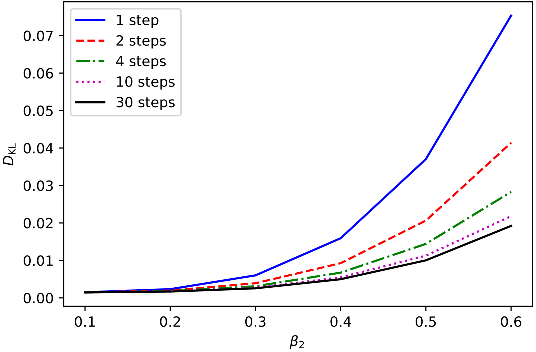
- Respecting sum rule important for maintaining fixed 1-body distribution
- If nominal short-range correlation doesn't satisfy, we add constant

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

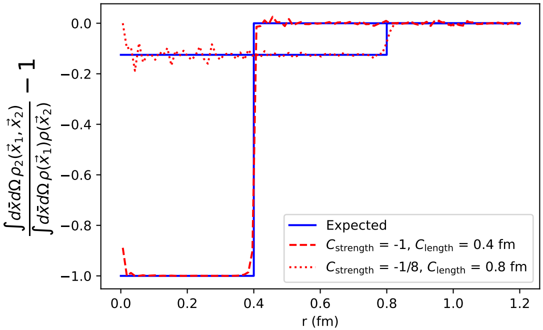
A natural way to compare probability distributions is the Kullback–Leibler (KL) divergence

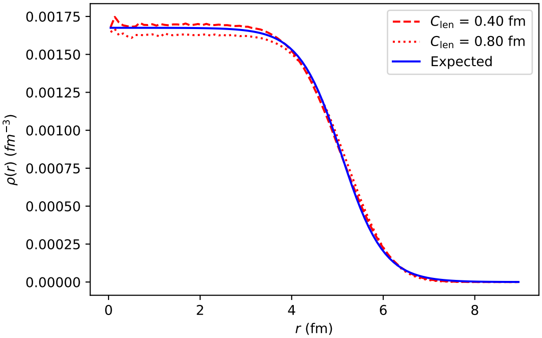
$$D_{\mathrm{KL}}(\rho_1||\rho_2) \equiv \int d^3x \rho_1(\mathbf{x}) \log \frac{\rho_1(\mathbf{x})}{\rho_2(\mathbf{x})}.$$

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



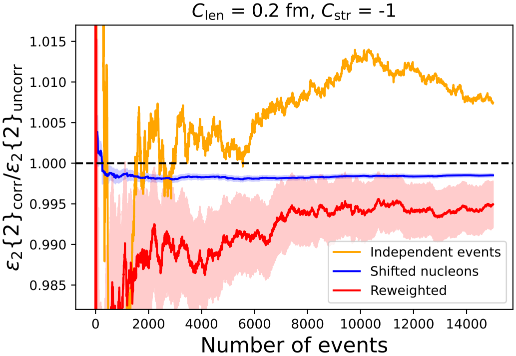
1- and 2-particle densities





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 $\Delta(C_{\mathrm{str}} C_{\mathrm{len}}^3) \gtrsim (0.3\text{ fm})^3$ 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 $C_{\text{strength}} \geq -1$

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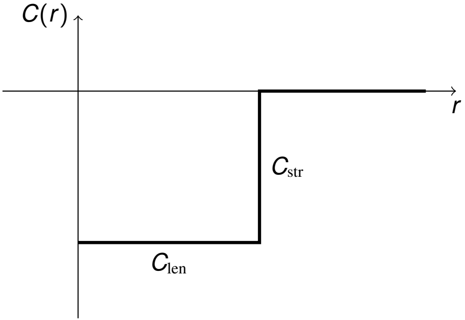

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