Constraining the input parameters of a transport+hydrodynamics model of heavy ion collisions in RHIC beam energy scan range with the help of Gaussian emulators

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Duke
UNIVERSITY

Outline

Probing QCD matter

Colliding heavy nuclei at relativistic energies

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Momentarily heating nuclear matter to extreme temperatures

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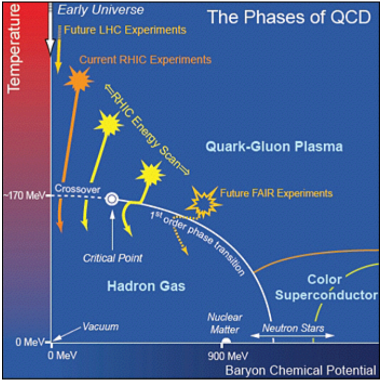
Deconfinement: Quark-gluon plasma



Relativistic Heavy Ion Collider (RHIC)

- Located at Brookhaven National Laboratory (NY)
- In operation since year 2000
- Au+Au and p+p collisions
- Collision energy $\sqrt{s_{NN}}$ varies from 7.7 GeV up to 200 GeV.
- Currently 2 active detectors: STAR and PHENIX

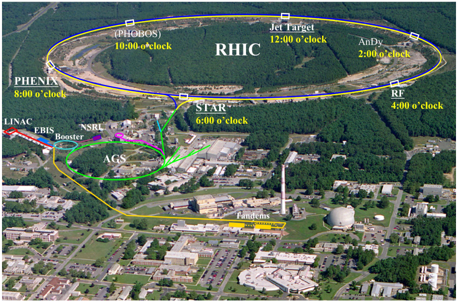
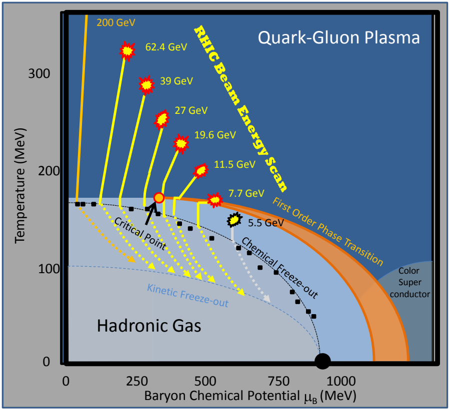


Image: https://hep-project-dphep-portal.web.cern.ch

RHIC beam energy scan

- Different collision energies probe different areas of the phase diagram of nuclear matter
- Baryochemical potential μ_B, related to the conservation of net-baryon number, becomes increasingly important at lower energies (nuclear stopping)
- $\mu_B \approx 0$ at 200 GeV and above; good for investigating temperature dependence of physical properties of the formed medium, such as viscosity (see J. Bernhard's talk from first week)



Picture: G. Odyniec, Acta Phys. Polon. B 43, 627 (2012).

RHIC beam energy scan

- Collision energy dependence of the physical parameters of the model ⇒ μ_B dependence
- Phase A: Find best-fitting model parameters for several collision energies independently
- If energy dependence observed in the best-fit parameters

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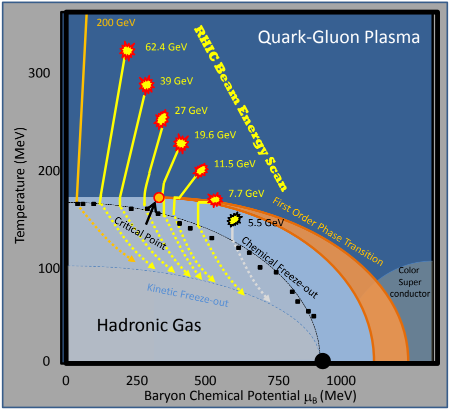
Phase B: parametrize the dependence and find the best fit over all collision energies simultaneously

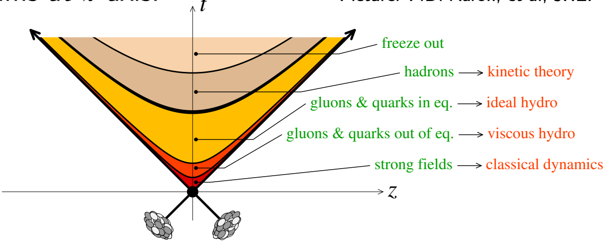


Picture: G. Odyniec, Acta Phys. Polon. B 43, 627 (2012).

Describing a heavy ion collision

Colliding beams at z-axis:

Picture: F.D. Aaron, et al, JHEP **1001**, 109 (2010).



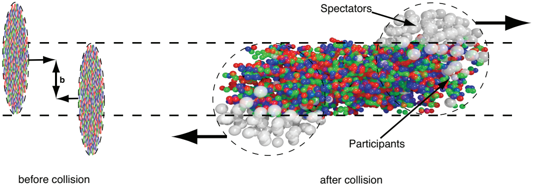
Milne coordinates:

- Proper time $\tau_0 = \sqrt{t^2 - z^2}$
- spatial rapidity $\tilde{\eta} = \frac{1}{2} \log \frac{t+z}{t-z}$

Kinematics:

- Momentum rapidity $y = \frac{1}{2} \log \frac{E+p_z}{E-p_z}$
- Pseudorapidity $\eta = \frac{1}{2} \log \frac{|\vec{p}|+p_z}{|\vec{p}|-p_z}$ (beam at $\eta = \pm\infty$)

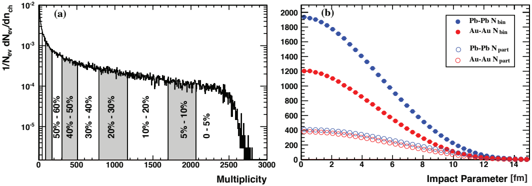
Collision centrality



R. Snellings, arXiv:1102.3010

Centrality classes quantify the estimated overlap of the colliding nuclei

- 0% - 5%: Head-on collision
- 20% - 30%: midcentral
- 60% - 80%: Peripheral



Elliptic flow v_2

Spatial anisotropy in initial state

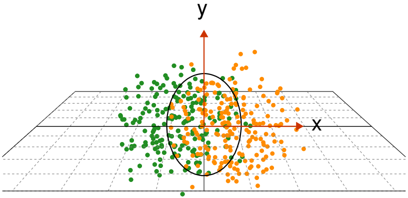
$\Downarrow$

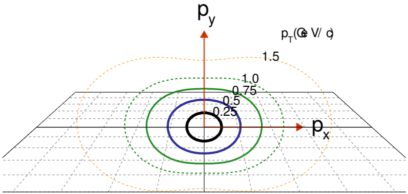
Pressure gradients

$\Downarrow$

Momentum anisotropy at final state:

$$E\frac{d^3N}{d^3p} = \frac{d^2N}{2\pi p_T dp_T dy}\left(1 + 2\sum_{n=1}^{\infty} v_n \cos[n(\phi - \Psi_{RP})]\right)$$

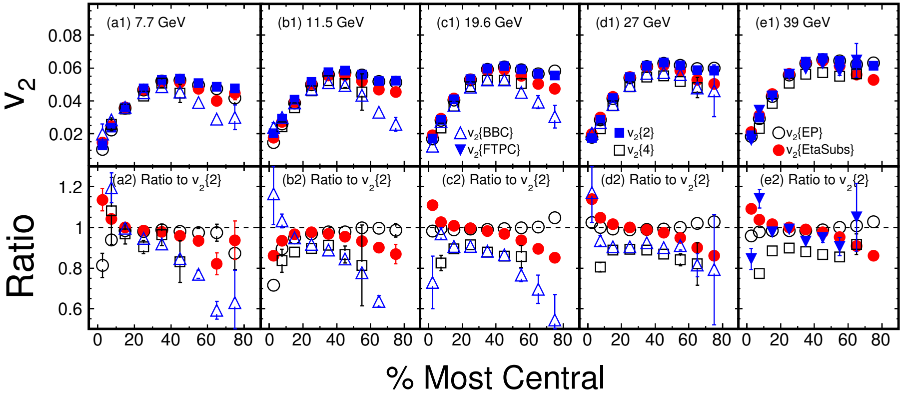




P. Sorensen, arXiv:0905.0174

Flow observables v_n imply collective behavior in the system

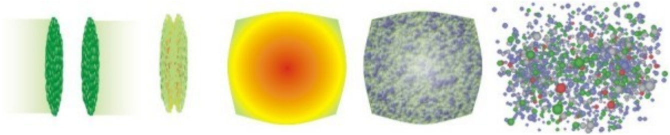
Elliptic flow v_2



L. Adamczyk *et al.* [STAR Collaboration], Phys. Rev. C **86**, 054908 (2012).

Hybrid model

Transport + hydrodynamics hybrid model



Source: S.A.Bass

Transport

- Microscopic description (point particles)
- Non-equilibrium evolution based on the Boltzmann equation

$$p^\mu \partial_\mu f_i(x,p) = C_i$$

- System consists of either quarks+gluons or hadrons

Hydrodynamics

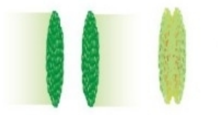
- Macroscopic description (energy/particle densities)
- Local equilibrium is assumed
- System evolves according to conservation laws

$$\partial_\mu T^{\mu\nu} = 0,\ \partial_\mu N^\mu = 0$$

- Transition from quark-gluon matter to hadronic matter described by the equation of state

Transport + hydrodynamics hybrid model

Karpenko, Huovinen, Petersen, Bleicher, Phys.Rev.C, 91, 064901 (2015)

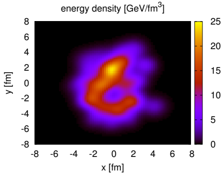


Initial state described by UrQMD[1] hadron transport

- Start the hydrodynamical evolution at time τ_0 when the two nuclei have passed through each other
- Convert energy, momentum and baryon number of each particle into 3D Gaussian distributions:

$$\Delta P^i = CP \exp\left(-\frac{\Delta x^2+\Delta y^2}{R_{\text{trans}}{}^2} - \frac{\Delta\tilde{\eta}^2}{R_{\text{long}}{}^2}\gamma_{\tilde{\eta}}^2 {\tau_0}^2\right)$$

$$\Delta N_B = CN_B \exp\left(-\frac{\Delta x^2+\Delta y^2}{R_{\text{trans}}{}^2} - \frac{\Delta\tilde{\eta}^2}{R_{\text{long}}{}^2}\gamma_{\tilde{\eta}}^2 {\tau_0}^2\right)$$

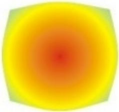


Karpenko et al., PRC91, 064901

- Add all Gaussians and map the resulting densities onto the hydro grid

[1] S. A. Bass *et al.*, Prog. Part. Nucl. Phys. **41**, 255 (1998), M. Bleicher *et al.*, J. Phys. G **25**, 1859 (1999).

Transport + hydrodynamics hybrid model



Hydrodynamical evolution

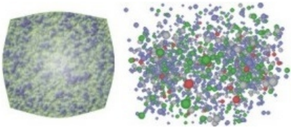
Karpenko et al., Comput. Phys. Commun. 185, 3016 (2014)

- (3+1)D viscous hydrodynamics with constant ratio of shear viscosity over entropy density η/s (bulk viscosity ignored)

$$\partial_{;\nu}T^{\mu\nu} = 0, \quad T^{\mu\nu} = (\epsilon + p)u^\mu u^\nu - pg^{\mu\nu} + \pi^{\mu\nu},$$
$$\partial_{;\nu}j^{\nu} = 0, \quad j^\mu = nu^\mu$$

$$\langle u^\alpha \partial_{;\alpha}\pi^{\mu\nu}\rangle = -\frac{1}{5}T\frac{\pi^{\mu\nu} - \pi^{\mu\nu}_{NS}}{\eta/s} - \frac{4}{3}\pi^{\mu\nu}\partial_{;\alpha}u^\alpha,$$
$$\pi^{\mu\nu}_{NS} = \eta\left[(\Delta^{\mu\alpha}\partial_{;\alpha}u^\nu + \Delta^{\nu\alpha}\partial_{;\alpha}u^\mu) - \frac{2}{3}\Delta^{\mu\nu}\partial_{;\alpha}u^\alpha\right]$$

Transport + hydrodynamics hybrid model



Freeze-out Procedure

- Transition from hydro to transport ("particlization") when energy density ϵ is smaller than critical value ϵ_C
- Construct 4-dimensional hypersurface σ with constant ϵ

"Cornelius" hypersurface finder, P. Huovinen and H. Petersen, arXiv:1206.3371.

- Particle distributions sampled according to the Cooper-Frye formula

$$p^0 \frac{N_i(x)}{d^3p} = d\sigma_\mu p^\mu f_i(p \cdot u(x), T(x), \mu_i(x))$$

- Rescatterings and final decays calculated in hadron transport (UrQMD)

Bayesian analysis

The modeling problem

Model parameters (input): $\vec{x} = (x_1, ..., x_n)$

$(\tau_0,\ R_{\text{trans}},\ R_{\text{long}},\ \eta/s,\ \epsilon_C)$

$\Downarrow$

Model output $\vec{y} = (y_1, ..., y_m) \Leftrightarrow$ Experimental values $\vec{y}^{\text{exp}}$

$(N_{\text{ch}},\ \langle p_T \rangle,\ v_2, ...)$

Goal: Find the "true" values of the input parameters, for which $\vec{x}^* \Rightarrow \vec{y}^{\text{exp}}$.
Determine the level of uncertainty associated with the proposed values

Bayes' theorem

Given a set $X = \{\vec{x}_k\}_{k=1}^{N}$ of points in parameter space and a corresponding set $Y = \{\vec{y}_k\}_{k=1}^{N}$ of points in observable space,

$$\boxed{P(\vec{x}^*|X, Y, \vec{y}^{\text{exp}}) \propto P(X, Y, \vec{y}^{\text{exp}}|\vec{x}^*)P(\vec{x}^*)}$$

- $P(\vec{x}^*|X, Y, \vec{y}^{\text{exp}})$ is the *posterior* probability distribution of $\vec{x}^*$ for given $(X, Y, \vec{y}^{\text{exp}})$
- $P(\vec{x}^*)$ is the *prior* probability distribution (simplest case: ranges of parameter values)
- $P(X, Y, \vec{y}^{\text{exp}}|\vec{x}^*)$ is the *likelihood* of $(X, Y, \vec{y}^{\text{exp}})$ for given $\vec{x}^*$ (to be determined with statistical analysis)

Likelihood function

$$P(X, Y, \vec{y}^{\,\mathsf{exp}} | \vec{x}^{*}) = \exp\left(-\tfrac{1}{2}(\vec{y}^{*} - \vec{y}^{\,\mathsf{exp}})^T \Sigma^{-1} (\vec{y}^{*} - \vec{y}^{\,\mathsf{exp}})\right),$$

where

- Σ is the covariance matrix.
  In this study $\Sigma = \text{diag}(\sigma_{\text{uc}}^2 \vec{y}^{\,\text{exp}})$, with σ_{uc} as a global estimate of relative uncertainty. Two values $\sigma_{\text{uc}} = 0.05$ and $\sigma_{\text{uc}} = 0.3$ tested, to check the sensitivity of results
- $\vec{y}^{*}$ is model output for the input parameter point $\vec{x}^{*}$

However:

1 hybrid simulation run requires $\approx$ 5 hours, 50 events produced

$\approx$ 100 000 events needed $\Rightarrow$ 2 000 runs

$\Rightarrow$ $\mathcal{O}(10^4)$ CPU hours for one evaluation of $\vec{y}^{*}$!

$\Rightarrow$ Need a way to predict model output for arbitrary input parameter point

$\Rightarrow$ Model emulation using Gaussian processes

Gaussian process

http://dan.iel.fm/george

Assumption: Set Y_a of values of observable y_a, corresponding to set X of points in parameter space, has a multivariate normal distribution:

$$Y_a \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\boldsymbol{\mu} = \mu(X) = \{\mu(x_1), ..., \mu(x_N)\}$ is the mean and

$$\boldsymbol{\Sigma} = \sigma(X, X) = \begin{pmatrix} \sigma(\vec{x}_1, \vec{x}_1) & \cdots & \sigma(\vec{x}_1, \vec{x}_N) \\ \vdots & \ddots & \vdots \\ \sigma(\vec{x}_N, \vec{x}_1) & \cdots & \sigma(\vec{x}_N, \vec{x}_N) \end{pmatrix}$$

is the covariance matrix with covariance function $\sigma(\vec{x}, \vec{x}')$.

Covariance function

Choice: Squared-exponential covariance function with a noise term

$$\sigma(\vec{x},\vec{x}') = \theta_0 \exp\left(-\sum_{i=1}^{n} \frac{(x_i - x_i')^2}{2\theta_i^2} \right) + \theta_{\text{noise}} \delta_{\vec{x}\vec{x}'}$$

The *hyperparameters* $\vec{\theta} = (\theta_0, \theta_1, ...\theta_n, \theta_{\text{noise}})$ are not known a priori and must be estimated from the given data

$\Rightarrow$ emulator training: Maximise the marginal likelihood (aka "evidence")

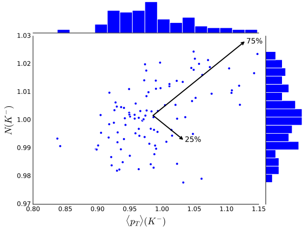
$$\log P(Y|X,\vec{\theta}) = \underbrace{-\frac{1}{2} Y^T \mathbf{\Sigma}^{-1}(X,\vec{\theta}) Y}_{\text{data fit}} \underbrace{-\frac{1}{2}\log|\mathbf{\Sigma}(X,\vec{\theta})|}_{\text{complexity penalty}} \underbrace{-\frac{N}{2}\log(2\pi)}_{\text{normalization}}$$

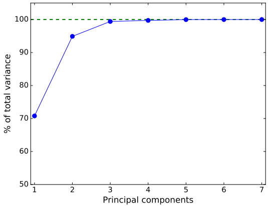
Principal component analysis

m observables $\Rightarrow$ m Gaussian processes

However, m can be up to $\mathcal{O}(100)$ at top RHIC energies and at the LHC!
Number of emulators can be reduced with principal component analysis:

- Construct orthogonal linear combinations of observables (= principal components) by performing an eigenvalue decomposition on the covariance matrix
- Eigenvalue λ_i represents the variance explained by principal component p_i
- Select the number of principal components which together explain desired fraction of total variance; often only a few PCs are needed to explain 99% of the variance





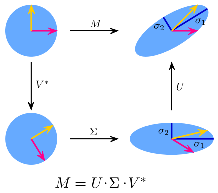
Singular value decomposition

N simulation points, m observables $\Rightarrow$ N x m data matrix Y

- Singular value decomposition:

$$Y = USV^T$$

  - S is a diagonal matrix containing the singular values
  - U and V^T are orthogonal matrices containing the left- and right-singular vectors, respectively



Wikipedia

- Eigenvalue decomposition of Y becomes

$$Y^TY = VS^2V^T$$

$\Rightarrow$ Singular values in S are square roots of eigenvalues of Y
$\Rightarrow$ Right singular vectors in V^T are eigenvectors of Y

Box-Cox transformation

Many times data is skewed; distribution peaks at values smaller or larger than mean

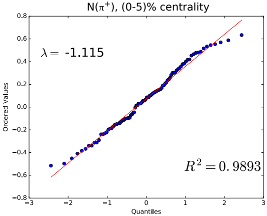
May affect the quality of principal component analysis

Try to fix the skew with Box-Cox transformation $y \to y^{(\lambda)}$:

G.E.P. Box and D.R. Cox, Journal of the Royal Statistical Society B, 26, 211 (1964)

$$y^{(\lambda)} = \begin{cases} (y^\lambda - 1)/\lambda & : \lambda \neq 0 \\ \log y & : \lambda = 0 \end{cases}$$

- y dimensionless $\Rightarrow$ Scale with experimental values y^{exp} first
- Assumes $y > 0$; shift if necessary
- Check against normal distribution after transformation (probability plot, QQ plot)



Markov Chain Monte Carlo

"emcee": D. Foreman-Mackey *et al.*, Publ. Astron. Soc. Pacific **125**, 306 (2013), arXiv:1202.3665

The posterior distribution is sampled with Markov Chain Monte Carlo (MCMC) method

- Random walk in parameter space, where each step is accepted or rejected based on a relative likelihood (calculated in terms of principal components)
- Converges to posterior distribution as number of steps $N \to \infty$
- Acceptance fraction a_f of steps measures the quality of random walk
  - $a_f \sim 0 \Rightarrow$ walker "stuck"
  - $a_f \sim 1 \Rightarrow$ purely random walk
  - aim for 0.2-0.5
- Autocorrelation time = Number of steps between independent samples "Burn-in" takes a few autocorrelations, gathering enough samples $\sim \mathcal{O}(10)$ autocorrelations

Analysis procedure

Scale with experimental values $\Rightarrow$ Unitless quantities of the order ($\mathcal{O}(1)$)

$\Downarrow$

Verify normal distribution of observables
(apply a transformation if necessary)

$\Downarrow$

Apply weights
Center the data

$\Downarrow$

Principal component analysis $\Rightarrow$ Determine required number of Gaussian processes

$\Downarrow$

Train the emulator(s)

$\Downarrow$

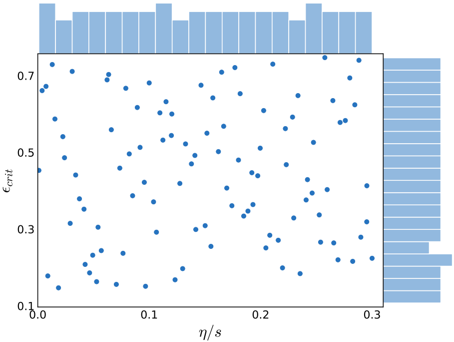
Calibrate on experimental data by running MCMC

Model results

Investigated parameter ranges

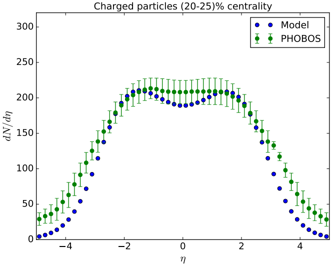
Sample points evenly over whole parameter space using Latin hypercube method

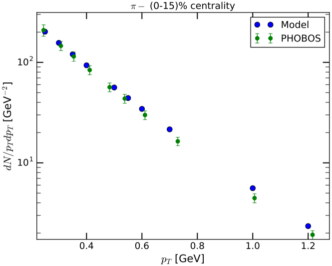
- Shear viscosity over entropy density η/s: 0.001 - 0.4
- Transport-to-hydro transition time τ_0: 0.4 - 3.1 fm
- Transverse Gaussian smearing of particles R_{trans}: 0.2 - 2.2 fm
- Longitudinal Gaussian smearing of particles R_{long}: 0.2 - 2.2 fm
- Hydro-to-transport transition energy density ϵ_C: 0.15 - 0.75 GeV/fm^3



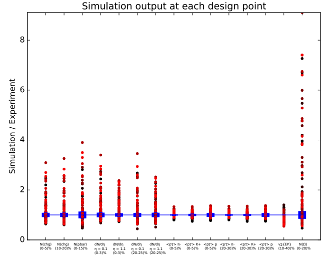
Investigated observables

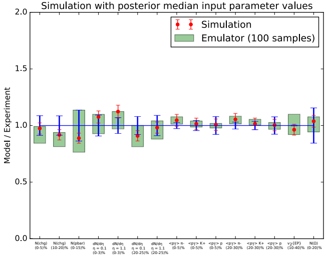
- Charged particles at midrapidity N_{ch}
- Charged particle pseudorapidity distribution $dN_{\text{ch}}/d\eta$
- Number of π, K, p, Ω at midrapidity
- Mean transverse momentum $\langle p_T \rangle$ for π, K, p
- Transverse momentum spectra dN/dp_T for π, K, p
- Charged particle elliptic flow $v_2\{\text{EP}\}$

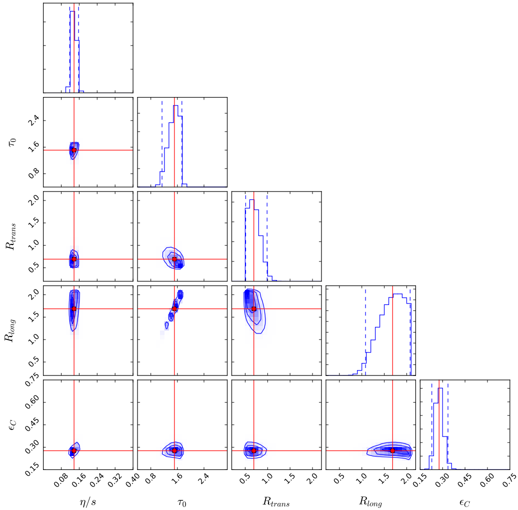




Results at 62.4 GeV, $\sigma_{\text{uc}} = 0.05$, weighted







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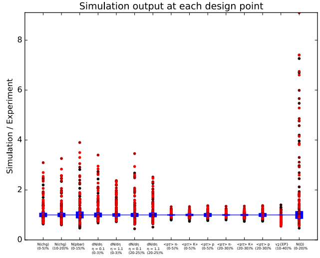
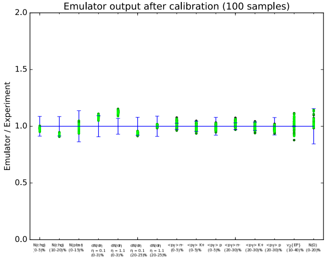
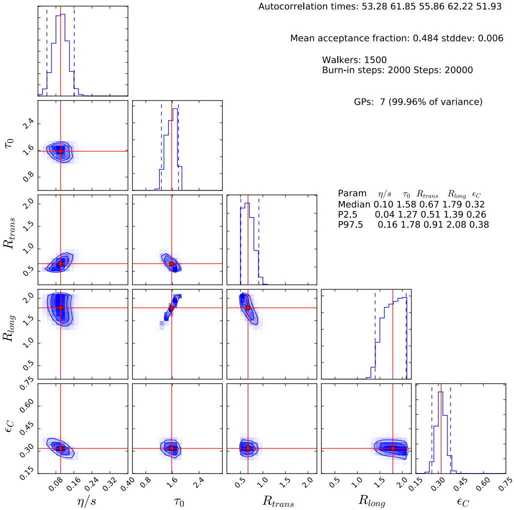
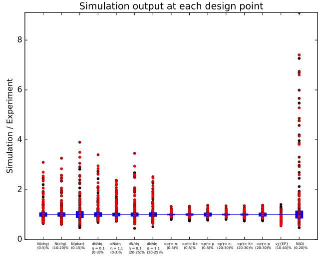
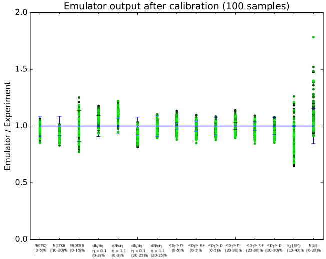


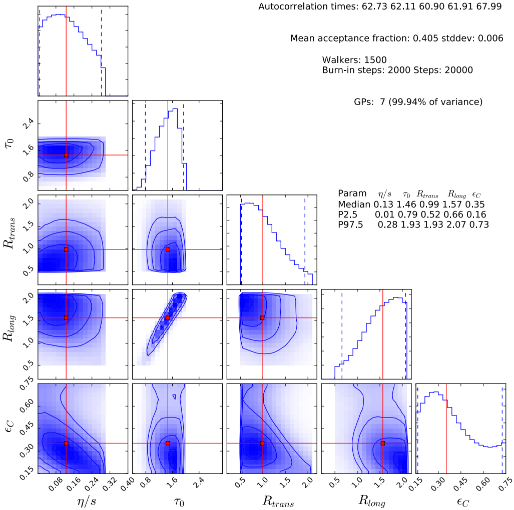




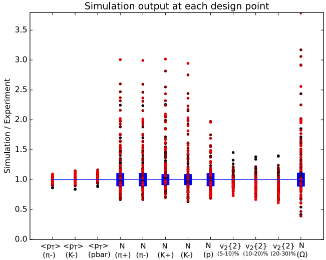
Results at 62.4 GeV, $\sigma_{\mathrm{uc}} = 0.30$

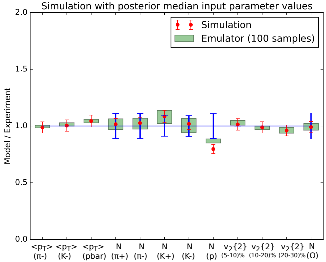


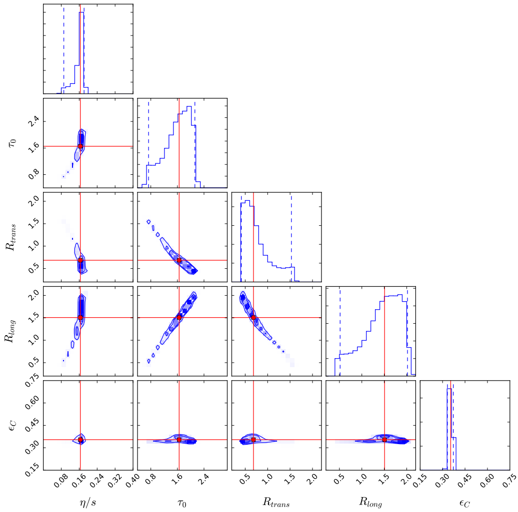




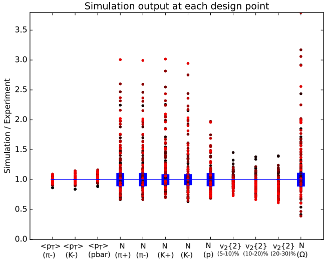
Results at 39 GeV, $\sigma_{\text{uc}} = 0.05$, weighted

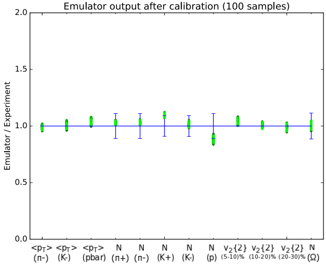


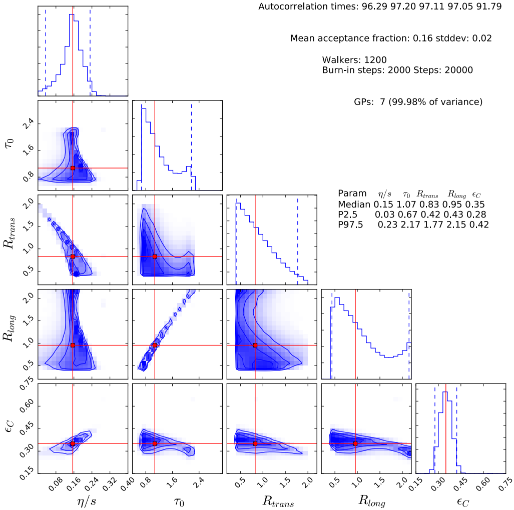




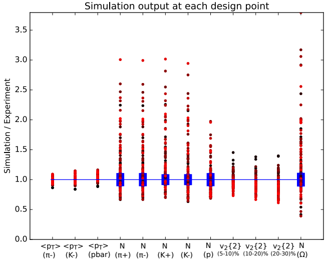
Results at 39 GeV, $\sigma_{\mathrm{uc}} = 0.05$

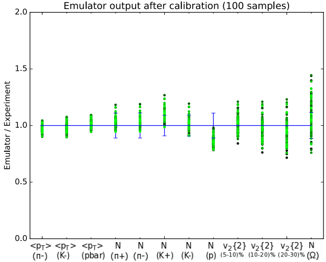


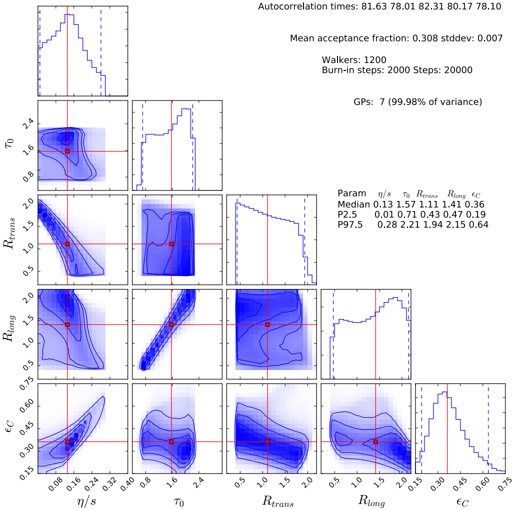




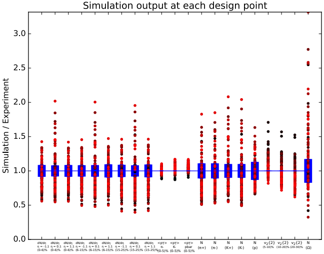
Results at 39 GeV, $\sigma_{uc} = 0.30$

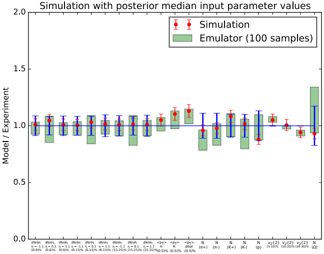


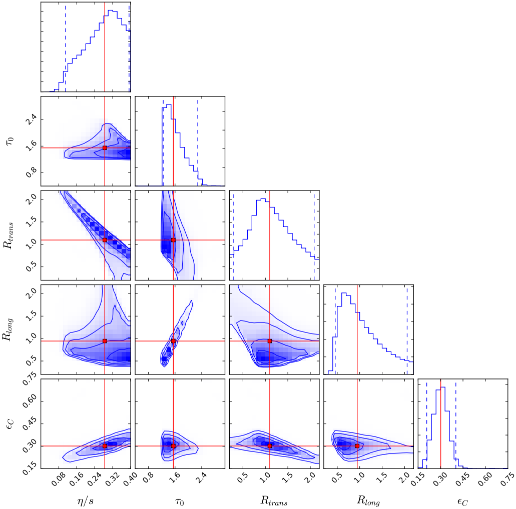




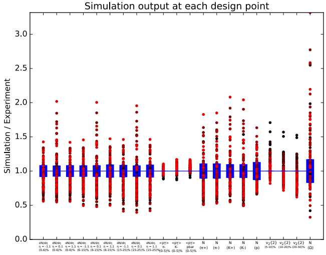
Results at 19.6 GeV, $\sigma_{\text{uc}} = 0.05$, weighted

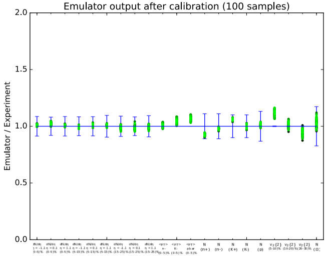


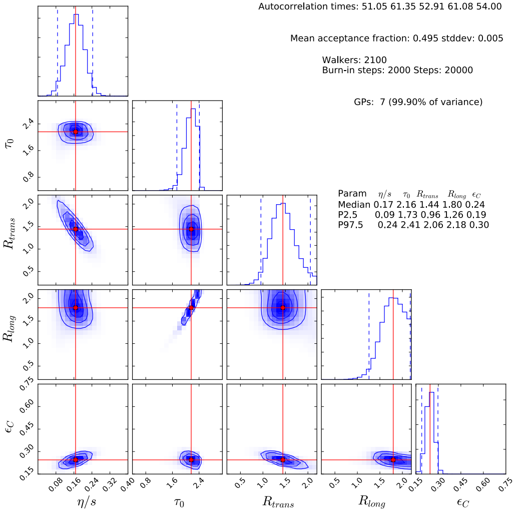




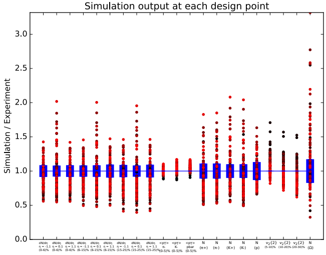
Results at 19.6 GeV, $\sigma_{\text{uc}} = 0.05$

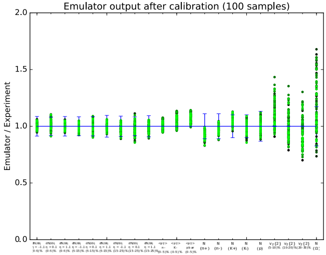


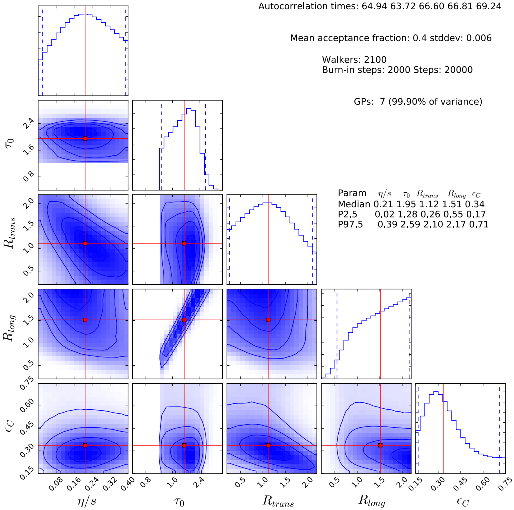




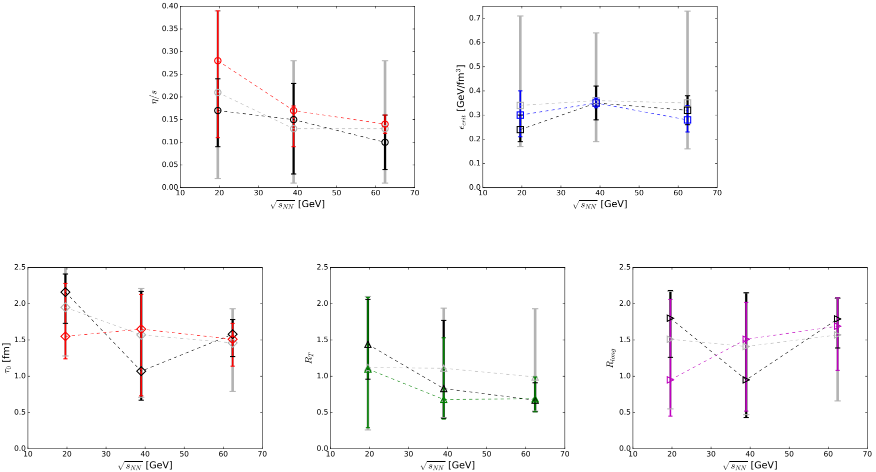
Results at 19.6 GeV, $\sigma_{uc} = 0.30$







Parameter dependence on collision energy



Summary

- Bayesian analysis provides a rigorous method for simultaneous estimation of both the best-fit values and the associated uncertainties for the parameters of heavy ion collision models
- Gaussian processes allow the emulation of complex models, making it possible to investigate multidimensional parameter spaces within reasonable computational effort
- Findings from the analysis of a transport+hydro+transport hybrid model:
  - Based on median values, η/s and transverse smearing factor R_{trans} have an increasing trend towards lower energies, while hydro-to-transport switching energy density ϵ_C is roughly constant with preferred value in the interval $\approx 0.2 - 0.4$ GeV/fm^3 (mainly constrained by $N(\Omega)$)
  - Hydro starting time τ_0 is either constant or increasing towards lower energies, while the longitudinal smearing factor R_{long} is either constant or decreasing at low energies. The two parameters are correlated and very sensitive to analysis parameters (weighting, uncertainty in likelihood)