Status Update: Simulations & distributed computing working group (SIMS-WG)

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JETSCAPE ANNUAL MEETING

BERKELEY, CALIFORNIA

JUNE 29, 2018

About SIMS-WG

- SIMS-WG was created about 3.5 months ago (March 10, 2018) with members at Ohio State University, Duke University, Brookhaven National Lab and Wayne State University. Members are:

Lipei Du, Derek Everett, Gojko Vujanovic, Ulrich Heinz (OSU)

Weiyao Ke, Jean-Francois Paquet, Steffen Bass (Duke)

Chun Shen (BNL)

Abhijit Majumder (Wayne State)

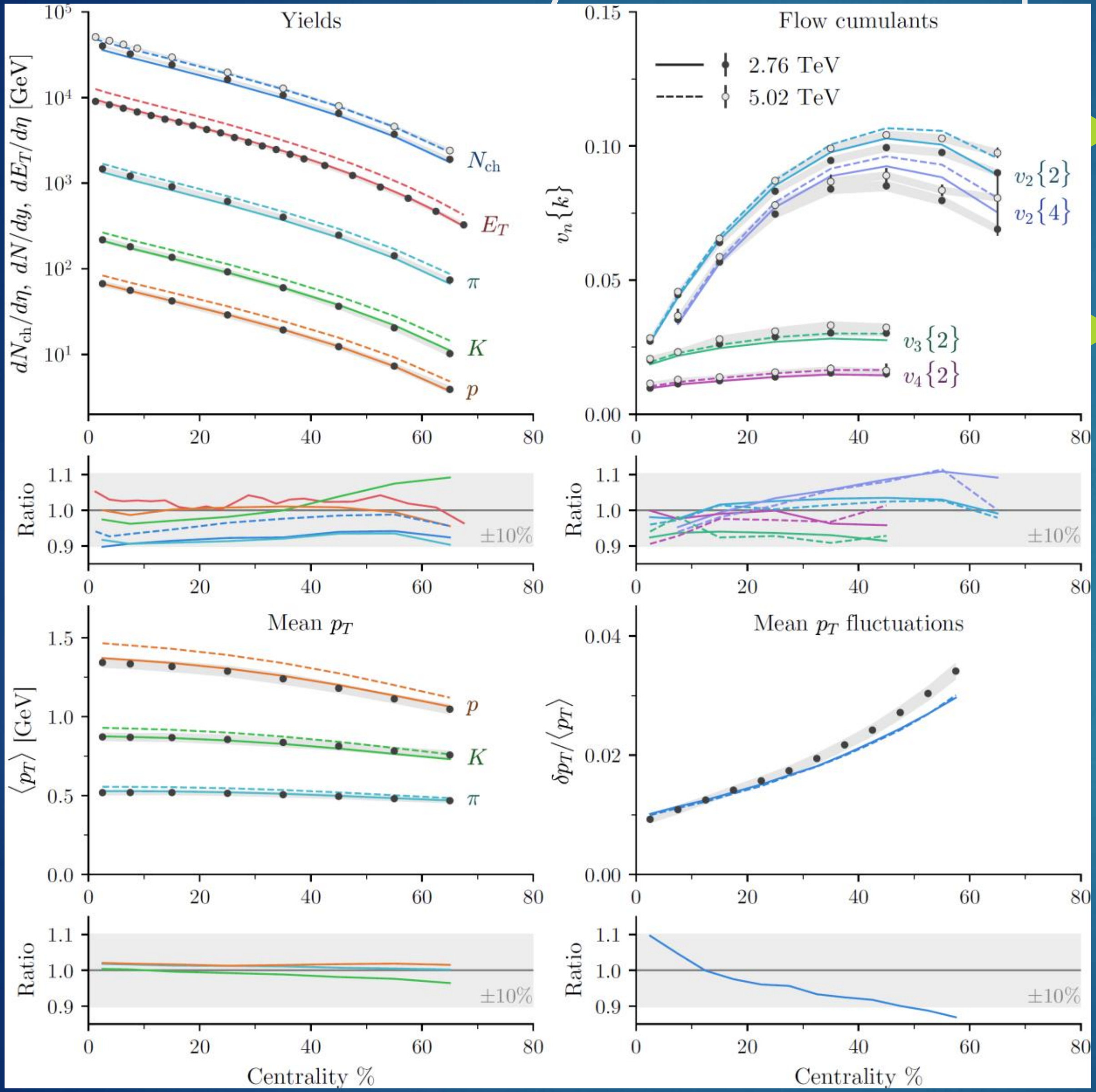
- SIMS is designed to bridge the gap between the various JETSCAPE groups, that is assist other working groups (e.g. PHYS, STAT) with large-scale simulations.
  - SIMS assists in optimizing the workflow of the JETSCAPE framework such that is scales well in High Performance Computing (HPC) environments.

First focus of the SIMS WG

- Jets are sensitive probes of the strongly-interacting medium, thus jet energy loss calculations need the best soft physics available.

- We have used the most recent parameters obtained from a Bayesian analysis by the Duke group of soft physics observables, to produce:
  - Simulations of Au-Au collisions top RHIC energy (200 GeV) and of Pb-Pb collisions at two LHC energies (2760 GeV and 5020 GeV).

Duke theory-data comparison



- A very good description of various soft observables
- Discrepancies between theorical calculation and data are ≲10%.

Figures from Jonah Bernhard's PhD thesis, arxiv:1804.06469

Modules used in simulations so far

- Using the best-fit parameters from the Bayesian Analysis performed at Duke (see arXiv:1804.06469), and their framework, SIMS produced 2+1D boost-invariant simulations on the Open Science Grid (OSG) consisting of:
  - TRENTO initial entropy density [PRC 92, 011901, 2015];
  - Free-streaming evolution [PRC 91, 064906, 2015] of the initial profile up to $\tau \sim$1.2 fm/c [arxiv:1804.06469];
  - Hydrodynamical evolution (OSU VISH 2+1D) including bulk and shear viscous pressure, was ran T_{ch} =151 MeV [PRC 91, 064906, 2015];
  - From T_{ch}, particle production is computed via Cooper-Frye. Note: UrQMD hadronic cascade evolution can be generated upon request.
  - Anisotropic flow (v_n), and event-plane angles (Ψ_n) of charged pions computed, needed for e.g. v_n of jets.
  - Hydro simulations are stopped below T_{ch}, at T_{kin}= 140 MeV, to allow for hydro estimate of possible jet energy loss after the hydrodymamical evolution (e.g. UrQMD).

The setup: OSG+OSiRIS

- A single 2+1D simulation is relatively inexpensive computationally, but lots of single-core simulations are needed.
- Open Science Grid (OSG) is ideal for distributed workload
  - 100+ sites in US
  - Universities & National Labs
  - Wide range of core count and core architecture per site

    − Difficult to predict execution time; not suited for multi-threaded jobs

    + Can continue running jobs at lower priority, if one runs out of allocation
- Results stored on Open Storage Research Infrastructure (OSiRIS)
  - Dedicated storage facility that all JETSCAPE members can access
  - Attached to other HPC infrastructures via high-speed backbone
  - Supports Globus: a research data management provider aware of the high-speed architecture ⇒ efficient data transfer to any local HPC facility used for jet energy loss calculations

2+1D Simulations produced for JETSCAPE

- On OSG, about 5,000 events were performed in a wide list of centrality classes (see backup slide for details)
- Also provided: 1 event-averaged simulation for testing of jet energy loss codes inside JETSCAPE framework
- Each optimized 2+1D simulation took <1.5 hours to complete on OSG
- Further optimizations were made to reduce disk usage (via e.g. HDF5 file formats)
- Results occupy 2TB of data stored on OSiRIS
- Stored on OSiRIS are:
  - Initial condition profiles, including binary collision density, for each event
  - Entire free-streaming + hydrodynamical evolution for each event
  - Entire freeze-out hypersurface for each event
  - Final (soft) hadron anisotropic flow (v_n), and event-plane angles (Ψ_n) for each event

Outlook

- Gearing up toward updating current events generated by SIMS-WG to 3+1D:
  - 3+1D TRENTO initial conditions (Duke) ✓
  - 3+1D Free-streaming (OSU) ✓
  - 3+1D Hydro (McGill ✓ OSU ✓)
  - SMASH hadronic transport ✓

✓: package incorporated into JETSCAPE
✓: package being developed/tuned before entering JETSCAPE

- Preparations under way with STAT/PHYS for Bayesian analysis of soft and hard observables using the JETSCAPE framework

- Applying for time on XSEDE to perform 3+1D Bayesian analysis; Stampede 2 at TACC needed for 3+1D simulations, more about this in Jean-François's talk

Backup Slides

Events simulated using current (Duke) best fit

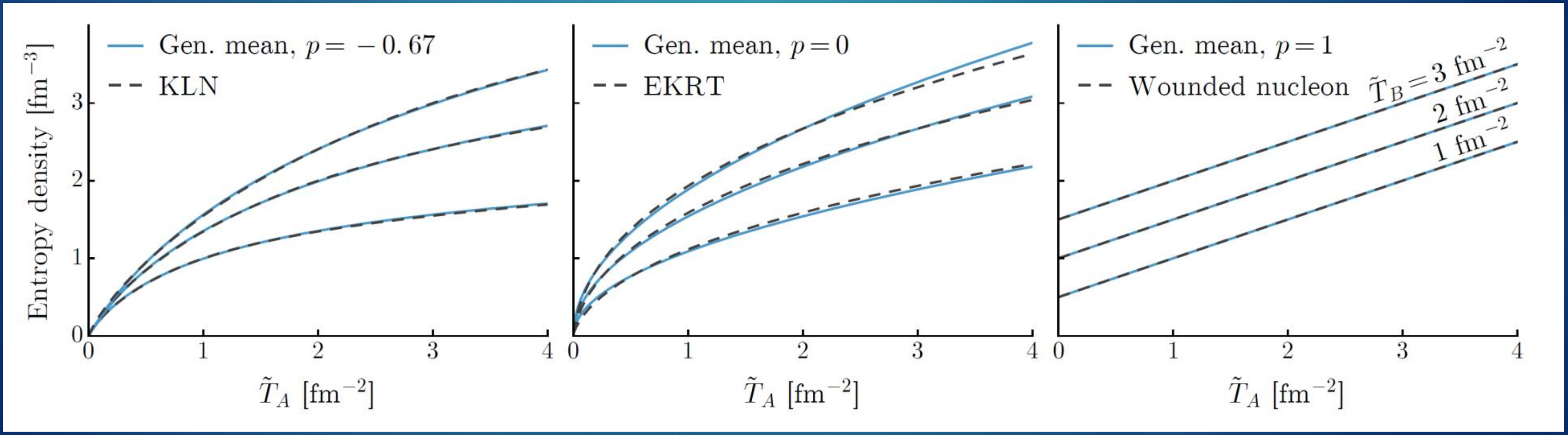
- List of centrality classes (at least 200 events per centrality class):
  - Au-Au $\sqrt{s_{NN}}$ = 200 GeV: 0-10%, 0-80%, 10-20%, 10-40%, 20-30%, 30-40%, 40-50%, 40-80%, 50-60%, 60-70%, Min Bias
  - Pb-Pb $\sqrt{s_{NN}}$ = 2760 GeV: 0-5%, 0-10%, 0-20%, 5-10%, 10-20%, 10-30%, 20-30%, 30-40%, 40-50%, 40-60%, 40-80%, 50-70%, 60-70%, Min Bias
  - Pb-Pb $\sqrt{s_{NN}}$ = 5020 GeV: 0-5%, 0-10%, 5-10%, 10-20%, 10-30%, 20-30%, 30-40%, 30-50%, 40-50%, 50-60%, 50-70%, Min Bias

About the models

- TRENTO is an *effective* model of the distribution at mid rapidity of the entropy density

$$\frac{dS}{dy} = N\left(\frac{T_A^p + T_B^p}{2}\right)^{\frac{1}{p}} = \begin{cases} \max(T_A, T_B) & p \to \infty \\ (T_A + T_B)/2 & p = 1 \\ \sqrt{T_A T_B} & p = 0 \\ 2T_A T_B/(T_A + T_B) & p = -1 \\ \min(T_A, T_B) & p \to -\infty \end{cases}$$

- $T_{A,B}$ is a participant nucleon density



Figures from Jonah Bernhard's PhD thesis on arxiv:1804.06469

About the models

- Both free-streaming and UrQMD solve the Boltzmann equation

$$p^{\mu}\partial_{\mu}f = C\{f\}$$

- The free-streaming model solves the collisionless Boltzmann equation, i.e. $C\{f\} = 0$
- UrQMD solves a system of Boltzmann equations (with collisions) for each hadronic species i

$$\sum_i p_i^{\mu}\partial_{\mu}f_i = C\{f_i\}$$

- In both cases, the conversion between the hydrodynamical degrees of freedom and particles is done via a distribution function

$$FS \rightarrow Hydro\colon T^{\mu\nu} = \int \frac{d^3p}{p}\ p^{\mu}p^{\nu}f \qquad Hydro \rightarrow UrQMD\colon E\frac{d^3N}{d^3p} = \int d^3\Sigma_{\mu}p^{\mu}f$$

$$T^{\mu\nu}u_{\nu} = \epsilon u^{\mu}$$

$d^3\Sigma_{\mu}$freeze-out surface elem.

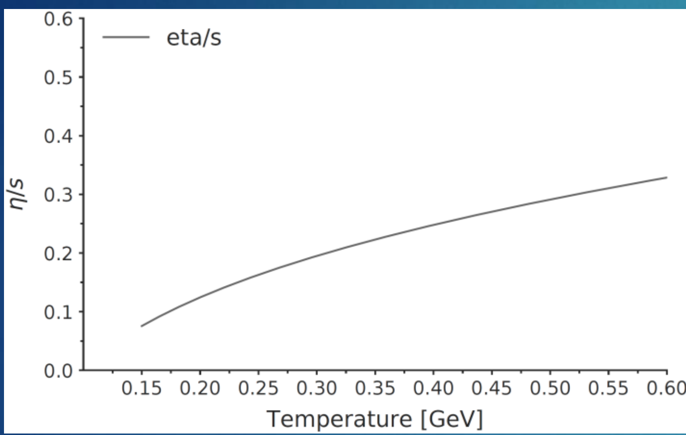
Viscous hydrodynamics & bulk pressure

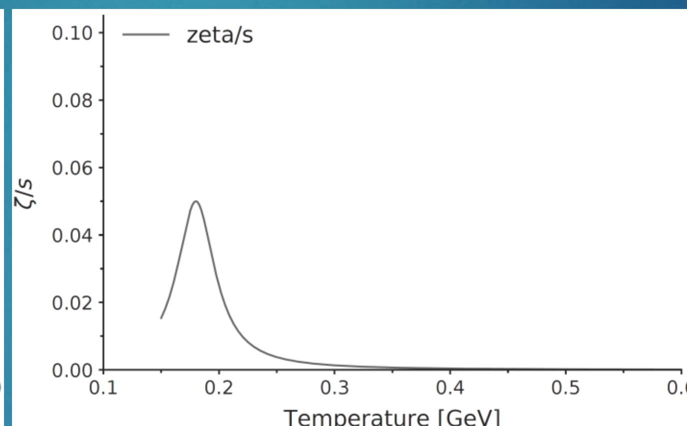
- Dissipative hydrodynamic equations :

$$\partial_\mu T^{\mu\nu} = 0 \qquad T^{\mu\nu} = T_0^{\mu\nu} + \pi^{\mu\nu} - \Delta^{\mu\nu}\,\Pi \qquad T_0^{\mu\nu} = \varepsilon u^\mu u^\nu - P\Delta^{\mu\nu}$$

$$\tau_\pi \dot{\pi}^{\langle\mu\nu\rangle} + \pi^{\mu\nu} = 2\eta\sigma^{\mu\nu} - \delta_{\pi\pi}\pi^{\mu\nu}\theta + \phi_7 \pi_\alpha^{\langle\mu}\pi^{\nu\rangle\alpha} - \tau_{\pi\pi}\pi_\alpha^{\langle\mu}\sigma^{\nu\rangle\alpha} + \lambda_{\pi\Pi}\Pi\sigma^{\mu\nu}$$

$$\tau_\Pi \dot{\Pi} + \Pi = -\zeta\theta - \delta_{\Pi\Pi}\Pi\theta + \lambda_{\Pi\pi}\pi^{\mu\nu}\sigma_{\mu\nu}$$





$\eta/s(T)$ and $\zeta/s(T)$ taken from Jonah Bernhard's PhD thesis on arxiv:1804.06469

- Other than ζ and η, all transport coefficients are in PRC **90** 024912 (2014).
- $P(\varepsilon)$: Lattice QCD EoS from Hot QCD collaboration [PRD 90, 094503 (2014)]

Duke Best-Fit

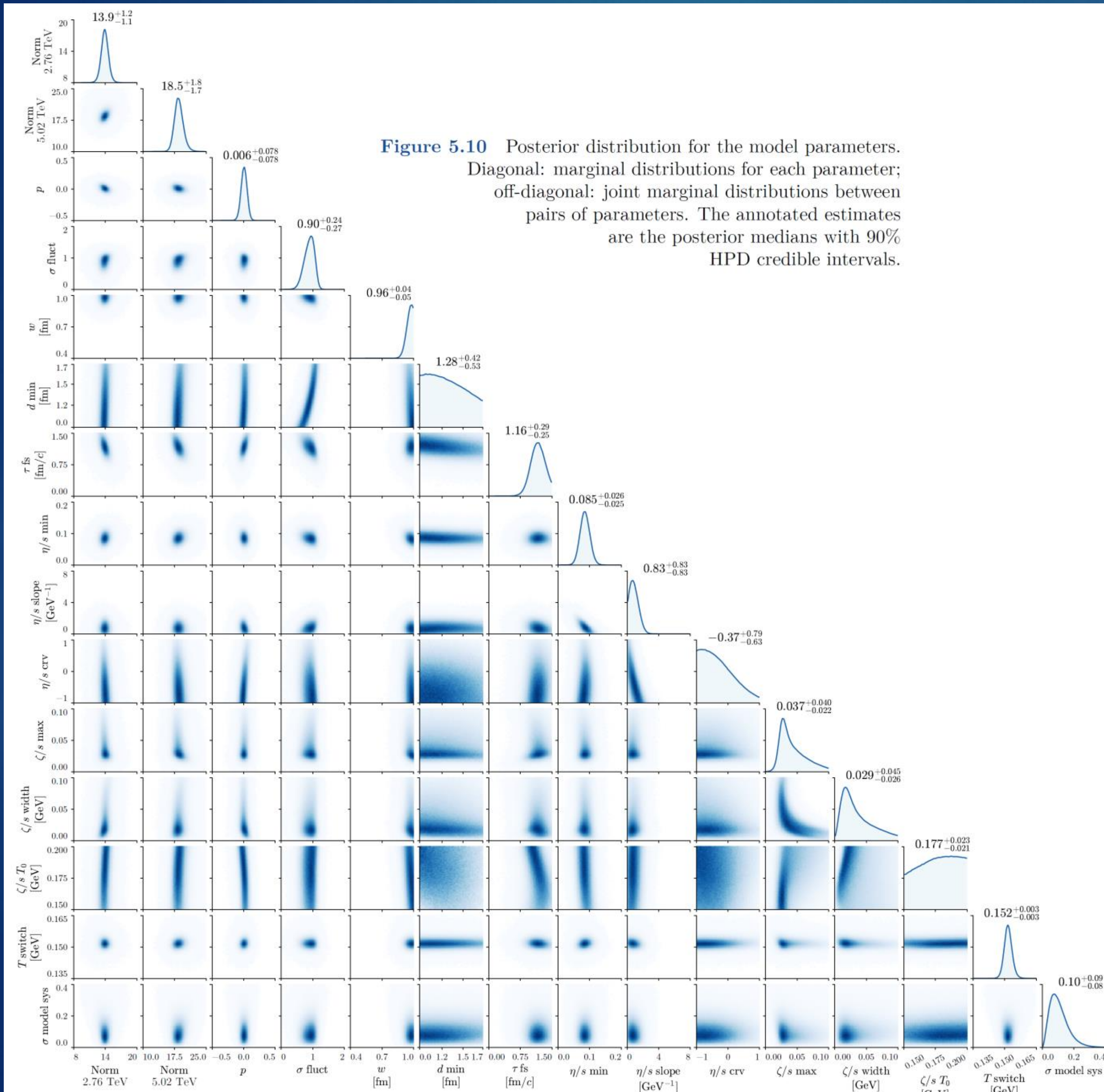


Figure 5.10 Posterior distribution for the model parameters. Diagonal: marginal distributions for each parameter; off-diagonal: joint marginal distributions between pairs of parameters. The annotated estimates are the posterior medians with 90% HPD credible intervals.

Figures from Jonah Bernhard's PhD thesis on arxiv:1804.06469