SIMS Working Group:
future plans

Conveners: **Jean-François Paquet** & Gojko Vujanovic

SIMS WG members:
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Abhijit Majumder (Wayne State)

JETSCAPE Collaboration Meeting
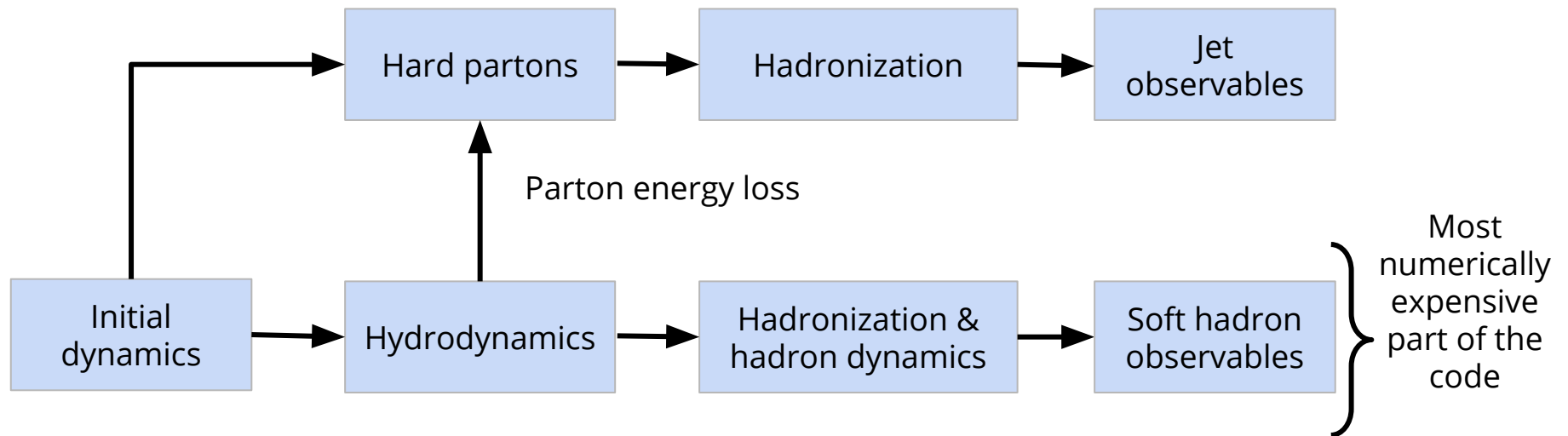Berkeley
June 29, 2018

Simulations and Distributed Computing (SIMS) Working Group
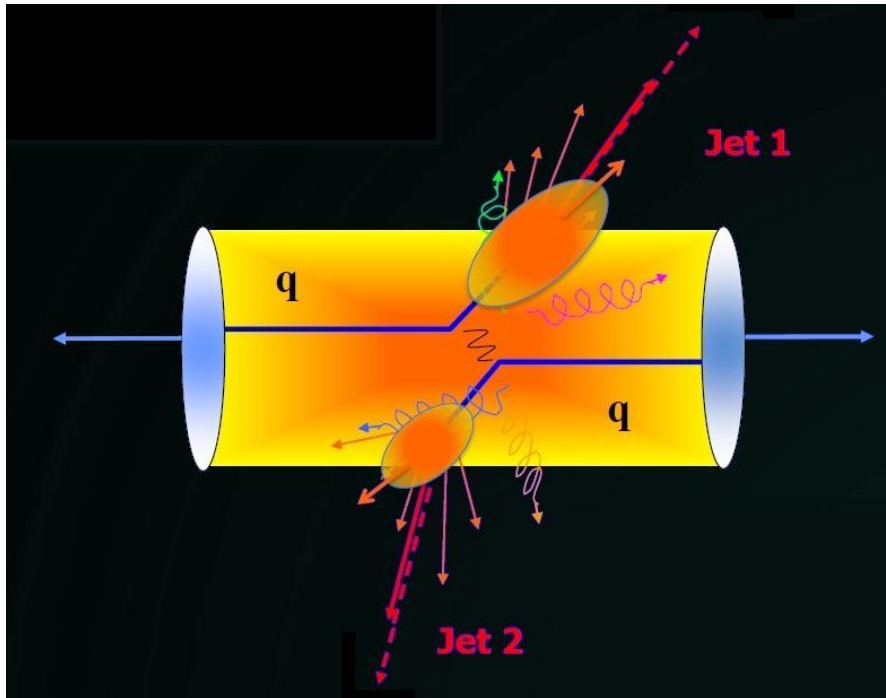
<u>Our responsibility:</u>

Carry out simulations over high performance computing facilities

<u>Current focus:</u>

Soft/hydrodynamic sector, the most **numerically expensive** part of the simulations (at the moment)
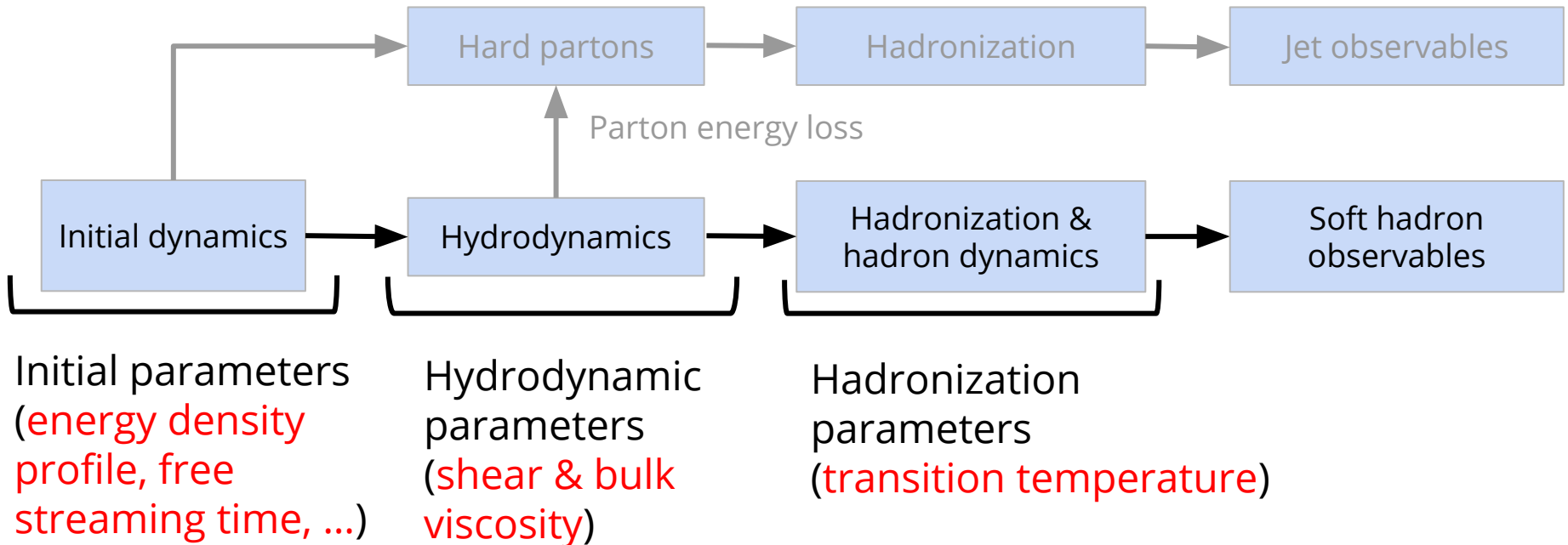
Soft physics simulation

(Modified from Xin-Nian Wang, QM2018)

Partons interact with the quark-gluon plasma

More realistic description of soft physics
(quark-gluon plasma)
leads to
more realistic calculation of
parton energy loss

[See e.g. Renk, Ruppert, Nonaka and Bass, PRC75:031902 (2007)]

Calibration & production of spacetime evolution

Initial parameters (energy density profile, free streaming time, …)

Hydrodynamic parameters (shear & bulk viscosity)

Hadronization parameters (transition temperature)

Two step process:
1) Calibrate model parameters to soft hadron data to find best set of model parameters
2) Use best set of model parameters to produce simulation of quark-gluon plasma spacetime evolution with which parton energy loss is then calculated
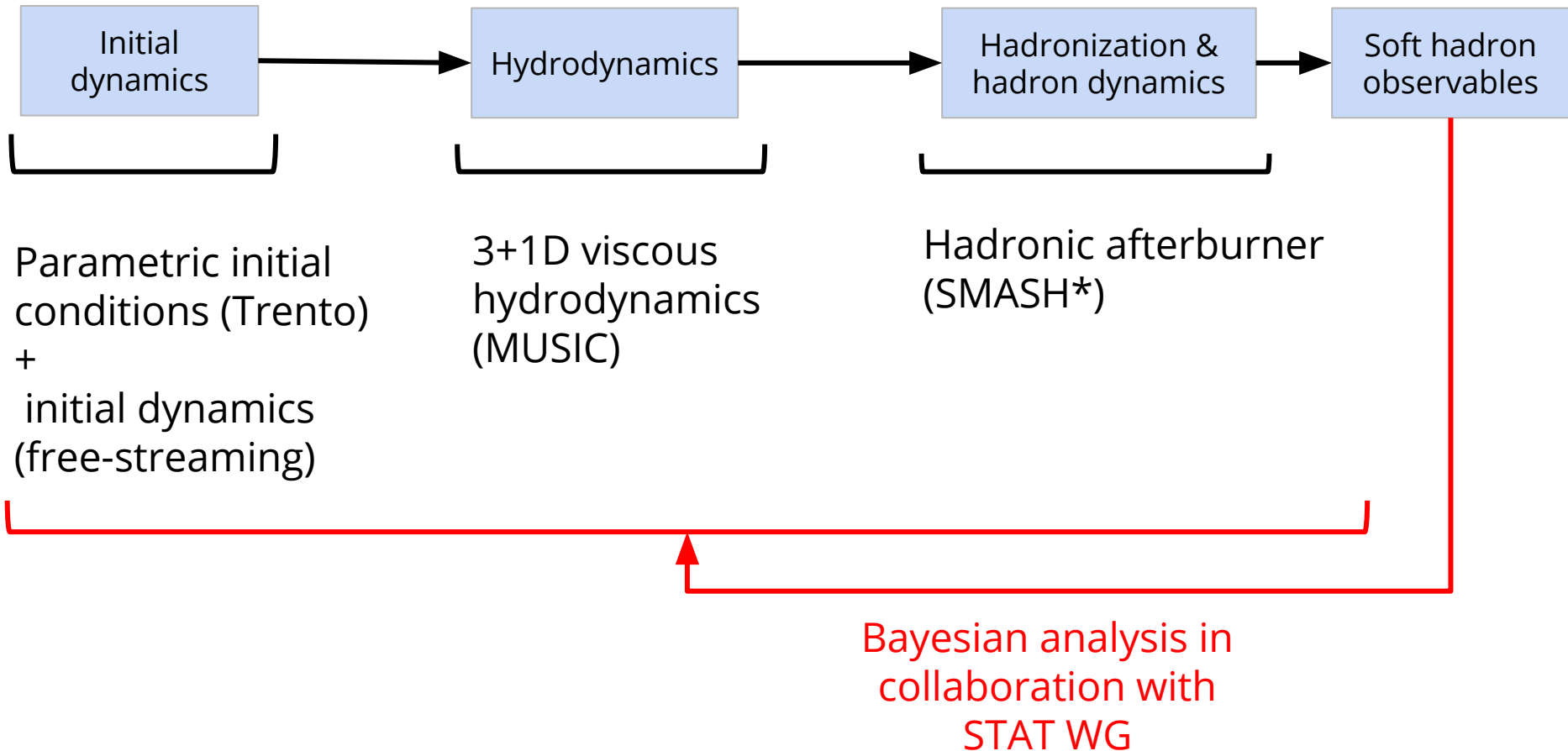
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Simulation of soft physics in JETSCAPE framework

Initial dynamics	→	Hydrodynamics	→	Hadronization & hadron dynamics	→	Soft hadron observables

Parametric initial conditions (Trento)
+
 initial dynamics (free-streaming)

3+1D viscous hydrodynamics (MUSIC)

Hadronic afterburner (SMASH*)
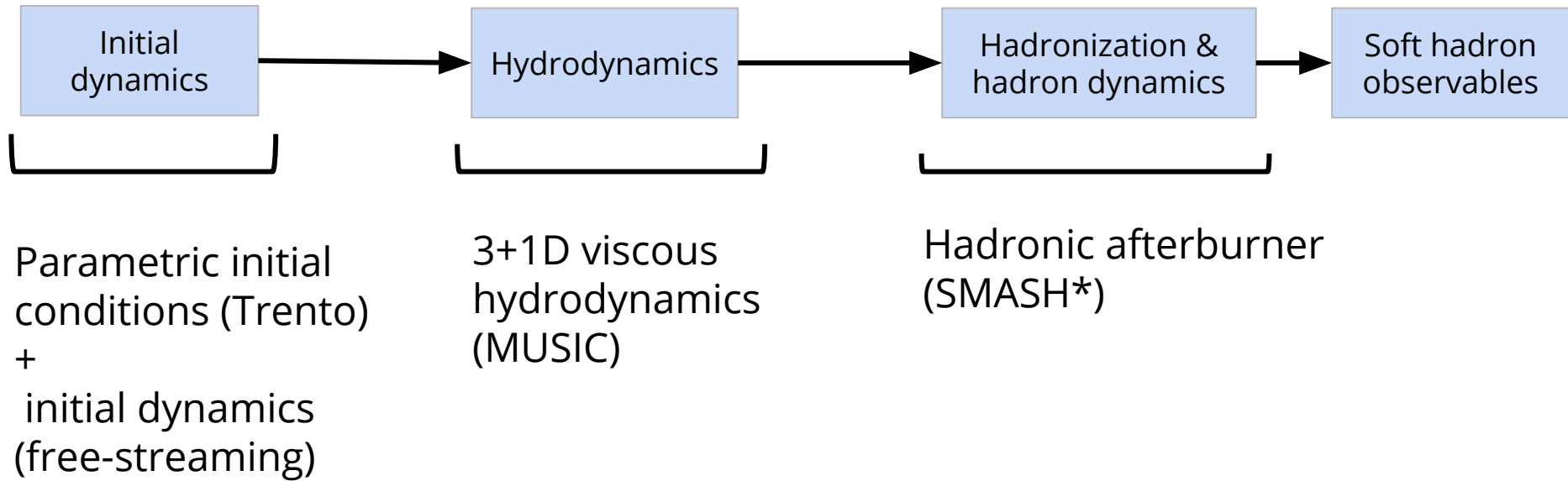
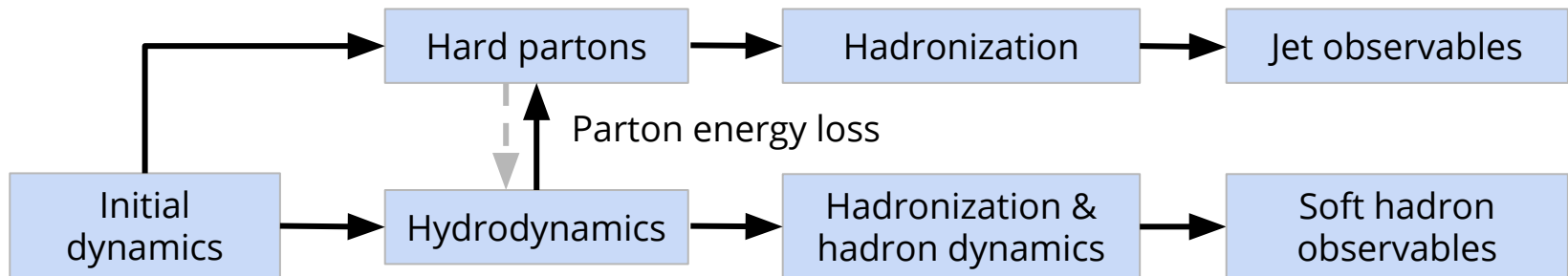JETSCAPE Framework will soon* have all the ingredients of a state-of-the-art hydrodynamic simulation of heavy ion collisions

* SMASH is currently being incorporated, c.f. COMP Working Group presentation

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Simulation of soft physics in JETSCAPE framework

Initial dynamics → Hydrodynamics → Hadronization & hadron dynamics → Soft hadron observables

Parametric initial conditions (Trento)
+
initial dynamics (free-streaming)

3+1D viscous hydrodynamics (MUSIC)

Hadronic afterburner (SMASH*)

Bayesian analysis in collaboration with STAT WG

SIMS/STAT collaboration: goals of first Bayesian analysis of soft sector

- Use JETSCAPE as self-contained simulation package for heavy ion collisions: **quark-gluon plasma simulation generated within framework**

- Take advantage of the combined **soft sector simulation in JETSCAPE** and **Bayesian analysis software and expertise** to perform analysis on soft hadron observables

- **Prepare for future analysis** where simultaneous soft/hard physics analysis is necessary (e.g. jet back-reaction into medium)

| Hard partons | → | Hadronization | → | Jet observables |

Parton energy loss

| Initial dynamics | → | Hydrodynamics | → | Hadronization & hadron dynamics | → | Soft hadron observables |

SIMS/STAT collaboration: short term objectives (1-3 months)

- **Complete development and validation** of soft physics sector of framework with COMP-WG

- **Benchmark JETSCAPE framework** and **apply for computer resources** to perform the Bayesian analysis

Application on **XSEDE computing resources** nearing completion

Performance of hydrodynamics (MUSIC) on parallel system
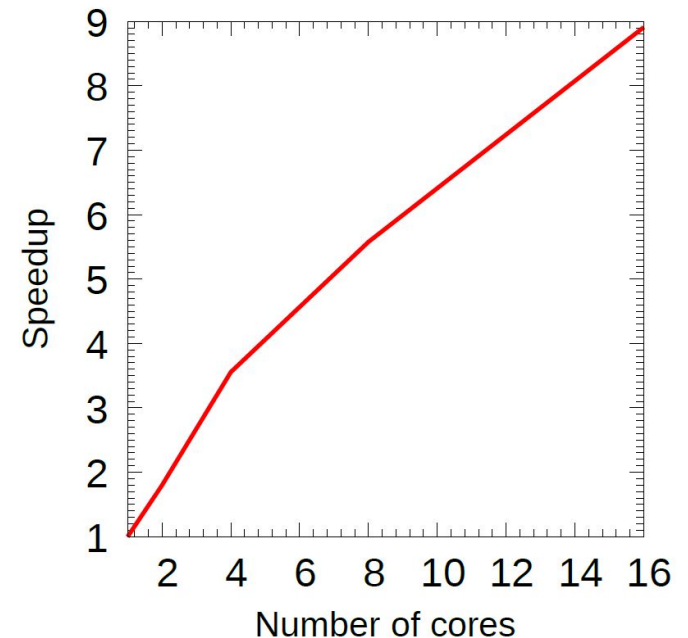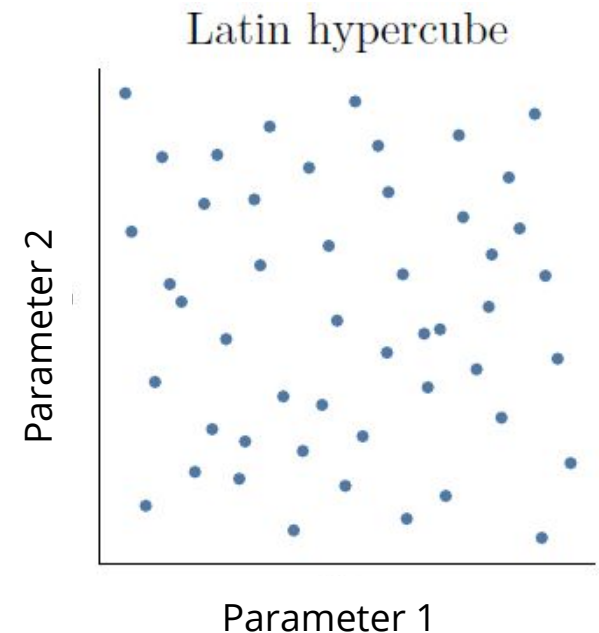
Bayesian analysis of soft sector & computer resources

A complete **Bayesian analysis** on the soft sector would have **~20 parameters**:
- Trento 2D (**initial condition** model) has **5** parameters. Trento 3D has **4** additional parameters.
- Flexible parametrization of the **temperature dependence of shear and bulk viscosity** requires **6** or more parameters
- **2 or 3** parameters for **free-streaming** & **particlization**
- One or two additional parameters per center of mass energy

To determine which **set of parameter best describe measurements**, we must **sample** a wide range of values of the **model parameters**.

10 to 40 samples per parameter should be used (Latin hypercube):
20 parameters × 10-40 samples = 200-800 parameter samples.

Latin hypercube

Parameter 2

Parameter 1

(Modified from Jonah Bernhard)

Bayesian analysis of soft sector & computer resources

- A **full 3+1D simulation of the soft sector** requires between **30 and 70 core-hours** (depending on the collision energy):
    - The 3+1D hydrodynamic simulation is the most resource intensive

- To compare with measurements, **1,000 to 5,000 full 3+1D hydrodynamic simulation of the soft sector per parameter sample** are required
    - Using a small number of hydrodynamic events (< 500) would require a pre-selection of initial condition events in centrality, and would results in non-negligible statistical uncertainty on certain observables

**Computer resource requirements per center-of-mass energy:**
30-70 core-hours × 1,000-5,000 × 200-800 = 6,000,000 to 280,000,000 core-hours

<u>A limited Bayesian analysis will be performed if computer resource allocated are insufficient for a full analysis</u>

May need to investigate using GPU-accelerated hydrodynamics for larger-scale analysis

Computer resource allocation request on XSEDE

- Considerable **CPU** needs**: 6,000,000 to 280,000,000 core-hours**
- Significant requirement in terms of memory (RAM): 25-100 GB for 3+1D soft sector simulations
  - Parallelization may be essential
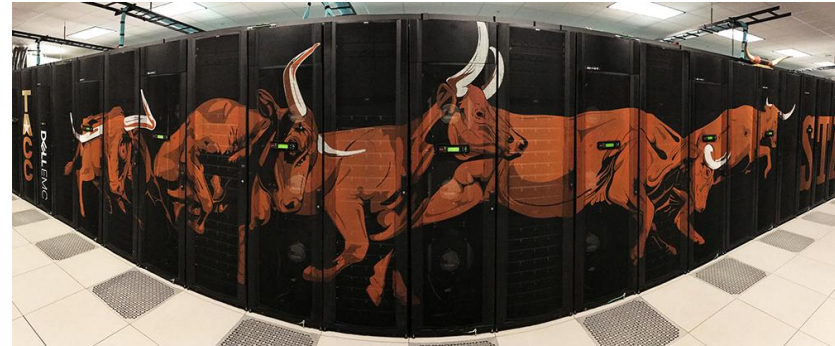
Time being requested on **Texas Advanced Computing Center (TACC)** flagship supercomputer: **STAMPEDE2**

Allocation request to XSEDE includes time needed for **Bayesian analysis of hard sector** as well (c.f. PHYS & STAT WG presentations)

Computer resources are requested on **Open Science Grid** since no need for large memory (RAM) or parallel capabilities

20,000,000 core-hours requested

SIMS/STAT collaboration: one year objectives

XSEDE (**computing resource**) allocation would begin

Separate Bayesian analysis of hard sector

Code development & validation in collaboration with STAT/PHYS/COMP

Generation of training data for emulator for 3+1D Bayesian analysis of soft sector

Perform 3+1D Bayesian analysis of soft sector

Produce 3+1D quark-gluon plasma for collaboration

Summer 2018   Fall 2018   Winter 2019   Summer 2019

Limited Bayesian analysis of soft sector with 2+1D hydrodynamics **for final validation**

Summary

- Simulations and Distributed Computing (SIMS) Working Group **focused on soft sector** for the coming year

- Close collaboration with COMP Working Group to **finalize soft sector part of the framework**

- Close collaboration with STAT Working Group to **perform Bayesian analysis of 3+1D simulation of soft sector** of heavy ion collisions

- Important short term goal: **apply for computing resources** for the analysis
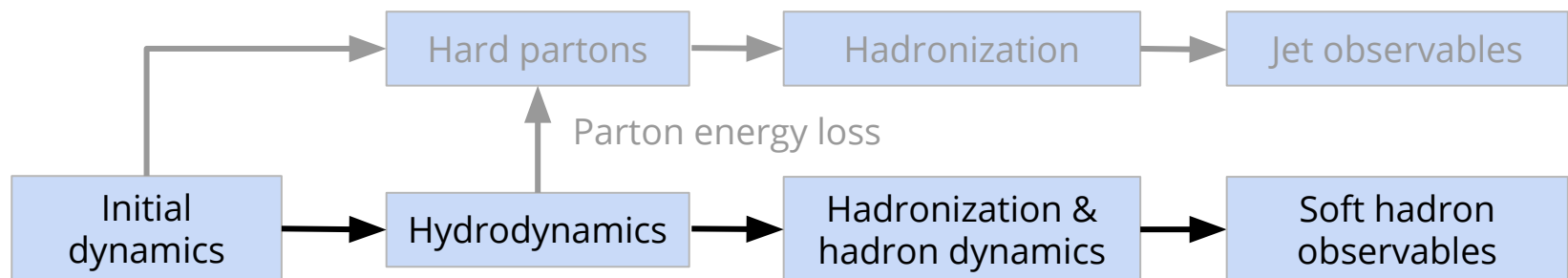
Back-up

SIMS/STAT collaboration: constraining the 3D quark-gluon plasma
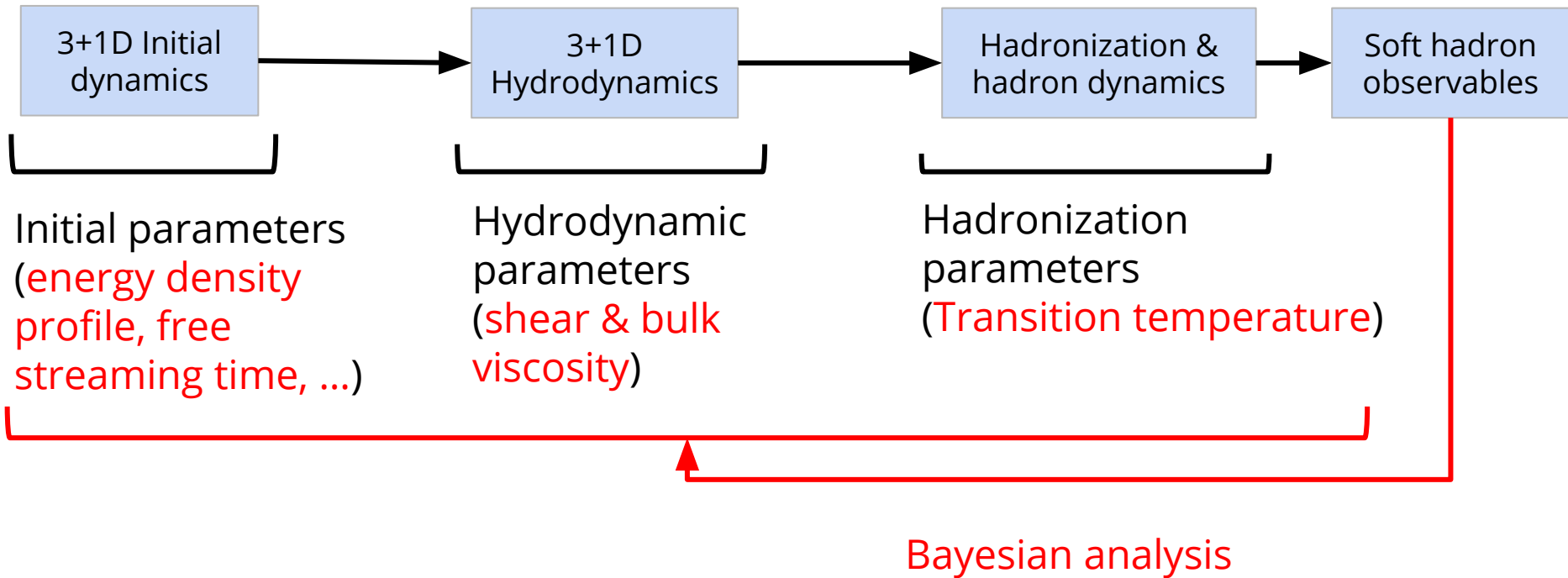
Systems: Pb-Pb 2760 GeV & 5020 GeV, Au-Au 200 GeV
Focus on p_T-integrated observables like in previous Bayesian analysis
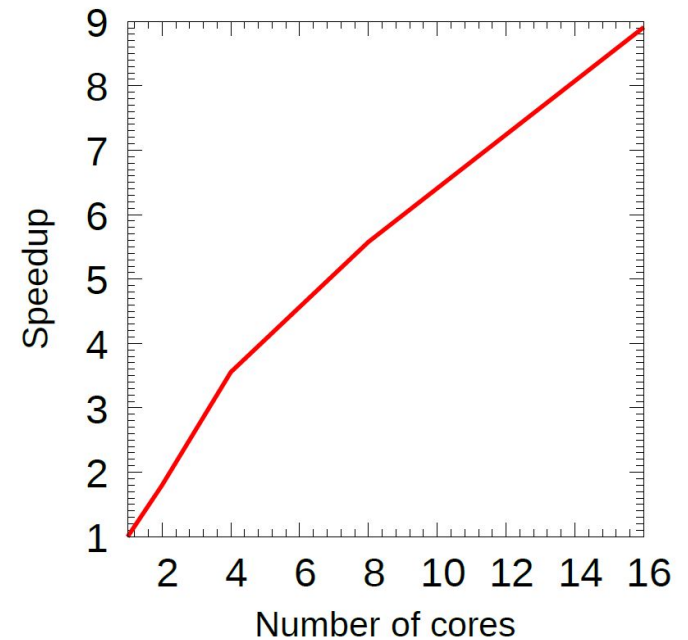
Additional parameters in 3+1D:
Four initial condition (Trento) parameters for rapidity direction

Trento 3D

Computing resources & benchmarking JETSCAPE

Benchmarking of all components of JETSCAPE framework to support applications for resource allocations on supercomputers

Benchmark of hydrodynamics (MUSIC) for parallel systems

The road ahead:
statistical analysis of soft hadrons with JETSCAPE

Previous **hydro medium not** produced with JETSCAPE code package and **best fit parameters** for hydro **not** obtained within JETSCAPE

Why do this with JETSCAPE?

- Necessary when jet back-reaction into medium is included
- To have a self-contained simulation package for heavy ion collisions

Challenges of doing this with JETSCAPE?

- No afterburner (yet)
- Possible overhead of studying soft physics with a hard-soft physics package (since no jet back-reaction at the moment)

Possible roadmap for coming months/years:
qualitative resource overview [can't quantify yet]

1. **Produce hydro medium with JETSCAPE** using current (Duke's) hydro parameters and validate (FS Duke vs FS OSU; VISH 2+1D vs MUSIC 2+1D)
    [Some human-hours]
2. Test & validate code to **calculate soft hadron observables** w/ JETSCAPE
    [More human-hours]
3. **Write code and wrappers** to better integrate calculation of soft hadron observables in JETSCAPE & match to Bayesian statistical analysis package
    [Lots of human-hours]
4. Perform a partial **Bayesian analysis** of soft observables using JETSCAPE with **2+1D hybrid simulation** (Trento+FS+hydro+SMASH)
    [Some human-hours & some amount of CPU-hours]
5. Perform a full Bayesian analysis of soft observables using JETSCAPE with **3+1D** hydrodynamics (Trento+FS+hydro+SMASH)
    [Lots of human-hours & lots of CPU-hours]

Bayesian analysis using JETSCAPE w/ 2+1D hydrodynamics

Why repeat Bayesian analysis using JETSCAPE in 2+1D hydrodynamics?

- To test that all scripts/code/wrappers are working
- Better estimates of required CPU-time and disk space usage for 3+1D
- Debugging/testing in 3+1D is very slow
- Possible different physics choices (e.g. δf)

Note: doesn't need to be full Bayesian analysis, can be a fast, limited one

Note: MUSIC and VISHNU
- Code essentially identical in terms of physics
- VISHNU is a 2+1D hydro code while MUSIC is a 3+1D hydro code (with 2+1D hydro mode): MUSIC is slower than VISHNU

Bayesian analysis using JETSCAPE w/ 3+1D hydrodynamics

Going to 3+1D implies

- More CPU-time [order 100], and more physical time [order 10, thanks to parallelization]
- More disk space usage [order 100]
- Slower and more complicated testing cycles
  [because longer run-time, tests may not be possible on local machines, ...]
- More parameters in the hydrodynamic model

Computer resources for 3+1D
Need to estimate CPU-time, RAM usage and disk space requirement to apply for appropriate computer resources for a large scale run

Timeframe

Tentative Timeframe
- Jun-Jul: complete testing & validation code for soft hadrons obs w/ JETSCAPE (no SMASH needed @ this time)
- June: Writing application for XSEDE allocation, i.e. need to have a CPU time estimate, RAM estimate, Disk space estimate (incl. SMASH).
- Jul-Sep: Close collaboration between COMP/PHYS and SIMS is needed to write all code/wrappers for Bayesian analysis incl. SMASH.
- Sep-Oct: Close collaboration between COMP/STAT and SIMS is needed to integrate JETSCAPE with Bayesian analysis software.
- Best if entire pipeline ready by mid October: XSEDE allocation would begin on Oct 1 (see for detail https://portal.xsede.org/allocations/research#xracquarterly)

Timeframe vs available manpower
- SIMS needs more jet quenching input