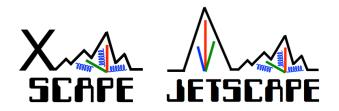


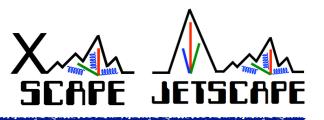
# If you have issues with installing/running JETSCAPE/X-SCAPE in Docker, ask questions/get support in slack channel:

## **#software-install-problems**



# Ask questions in slack channel: #july17-18-xscape-framework

## JETSCAPE/X-SCAPE



## **Event generator**

 A *framework* for general-purpose MC event generators in e-A, p/d-A and A-A collisions

## **Statistical toolkit**

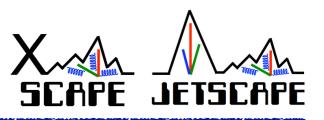
 Extract model parameters via Bayesian analysis with Gaussian Process Emulators

https://github.com/JETSCAPE/X-SCAPE

https://github.com/JETSCAPE/STAT



A general-purpose MC framework  $X_{\text{sc}}$ 



### JETSCAPE/X-SCAPE is not just for jets! It is a framework for *general-purpose* event generators

#### The JETSCAPE/X-SCAPE framework is modular

The core framework decides how physics modules can interact with each other — but the modules themselves can be user-contributed



#### Physics modules are open-source

Key improvement in particular in heavy-ion physics predictions can be checked against many observables simultaneously

### A unified framework has clear benefits when we want to compare models of one particular part of a multi-stage event evolution

## The current status

latessa Merge pull request #3 from JETSCAPE/ip-glasma-docs JetScapeDoxy.conf Change from XML Master file Main file .github/workflows merging public main with 1. README.md updated version number to cmakemodules Remove not needed C README LINUX.md config docker updated docker files to include PYTHIA8 env variable activate\_jetscape.sh Merge ReleaseAApaper into master (features from 2.0, QM2019 de... examples refactor of PythialsrMusic and fix of typo E READINE Packages updated IP-Glasma instructions ß Merge pull request #101 from JETSCAPE/3DGlauber-MUSIC-FOR\_... JETSCAPE 3.5.4 https://github.com/JETSCAPE/JETSCAPE .gitignore The JETSCAPE simulation framework is an overarching computational envelope for developing complete event generators for heavy-ion collisions. It allows for modular incomparation of a wide wariety of existing and future software that simulates different aspects of a heavy-ion collision. For a full introduction to JETSCAPE, please Compile PythialsrMUSIC only when turn on 3DGlauber, MUSIC and ... cMakeLists.txt see The JETSCAPE framework. CONTRIBUTING.md Mention that ideally one should use doxygen code comments in he... Please cite The JETSCAPE framework if you use this package for scientific work. Updated COPYING COPYING Installation Update JetScapeDoxy.con Pleasense the Installation Instruction @reate LICENSE README.md changed README to point to X-SCAPE wiki instead of JETSCAPE ∃ README.md

#### The framework(s) are available and ready for public use

Wide variety of physics available — additions ongoing

Ideal time to contribute additional physics modules

#### X-SCAPE 1.0

#### https://github.com/JETSCAPE/X-SCAPE

The X-ion collisions with a Statistically and Computationally Advanced Program Envelope (X-SCAPE) is the enhanced (and 2nd) project of the JETSCAPE collaboration which extends the framework to include small systems created in p-A and p-p collisions, lower energy heavy-ion collisions and electron-lon collisions. The new framework allows for novel functionality such as the ability of the main simulation clock to go backwards and forwards, to deal systematically with initial state and final state evolution. It allows for multiple bulk event generators to run concurrently while exchanging information via a new Bulk Dynamics Manager. The X-SCAPE framework can be run using the new functionality or in JETSCAPE mode allowing for full backwards compatibility. New modules can also run in a hybrid fashion, choosing to use or not use the new clock functionality. More documentation of the new X-SCAPE framework capabilities will be provided in the near future. For now, test examples showcasing the new X-SCAPE framework functionalities can be found in the ./examples/custom\_examples/ directory (for example in PythiaBDMTes.cc and PythiaBrickTest.cc).

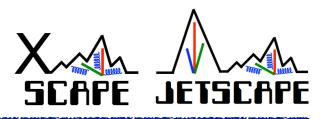
The JETSCAPE simulation framework is an overarching computational envelope for developing complete event generators for heavy-ion collisions. It allows for modular incorporation of a wide variety of existing and future software that simulates different aspects of a heavy-ion collision. For a full introduction to JETSCAPE, please see The JETSCAPE framework.

Please cite The JETSCAPE framework if you use this package for scientific work.

#### JETSCAPE 2023 Online School

X-S

D



 X-SCAPE is fully backwards compatible to JETSCAPE!
 → X-SCAPE 1.0 includes and can be run in JETSCAPE mode exactly like JETSCAPE 3.5.x !

#### **JETSCAPE** release map:

- 3.6.x last feature/physics release (fragmentation hadrons in SMASH)
- 4.x code optimization

### **X-SCAPE release map:**

- 1.1 to include JETSCAPE 3.6.x
- 2.x Low beam energy AA
- 3.x EIC physics

In this lecture, if I refer to JETSCAPE (logo in upper right corner), I refer to running X-SCAPE 1.0 in JETSCAPE mode!

If I refer to X-SCAPE (logo in upper right corner), I refer to X-SCAPE 1.0 specific functionalities not part of JETSCAPE





#### JETSCAPE / X-SCAPE JINSTALLING X-SCAPE Note: State of the state of t

Joern Putschke, WSU

code

Q Type []	to search
-----------	-----------

🕑 Security 🗠 Insights 🕸 Settings



8

Doo Installation I

#### https://github.com/JETSCAPE/X-SCAPE/wiki/Doc.Installation **Doc.Installation** Joe Latessa edited this page on Apr 11 · 5 revisions **Doc.Installation** To run X-SCAPE, you will need to install several software pre-requisites, and then build X-SCAPE. Acquiring the prerequisites using a container environment will be simpler than installing the pre-requisites manually. Find a page... Instructions to Install and Run X-SCAPE Using Docker Preferred for local use and development Home We recommend to install X-SCAPE and its pre-requisites using Docker. **3DGlauber, MUSIC, iSS** Usually needed to use container Instructions to Install and Run X-SCAPE Using Singularity feature in large computing farms **Doc.FAQ** Another option is to install X-SCAPE and its pre-requisites using Singularity. (some comments later) **Doc.Installation** Manual Installation (not recommended) Please see the instructions here. **External packages** To run certain external software (MUSIC, CLVisc, SMASH), you will need to explicitly download them, and you may need to re-run cmake with specific command-line options. Scripts to download and install the external packages are provided in external\_packages/. Please see external packages for full details. **Doc.Installation.Docket** The available cmake options are: **Doc.Installation.Docket** cmake .. -DUSE\_MUSIC=ON -DUSE\_ISS=ON -DUSE\_FREESTREAM=ON -DUSE\_SMASH=ON -DUSE\_CLVISC=ON **Doc.Installation.Docket Doc.Installation.Docket** Doc.Installation.Docker

JETSCAPE 2023 Online School

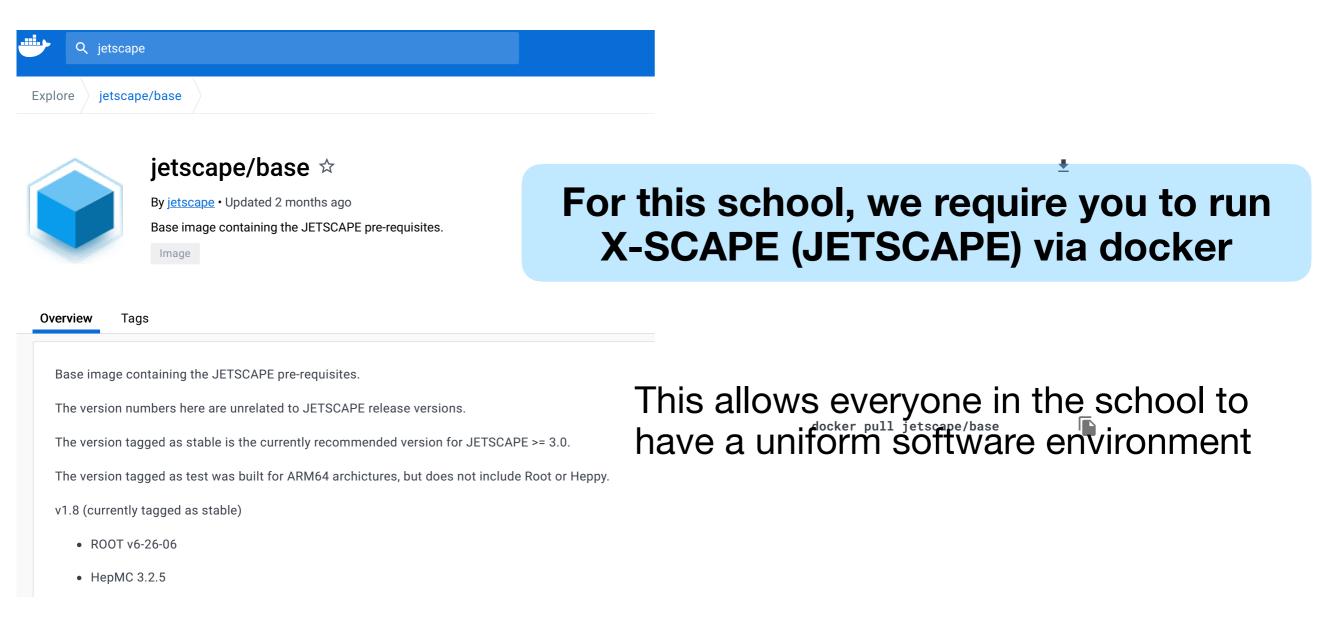
# **Installing X-SCAPE**



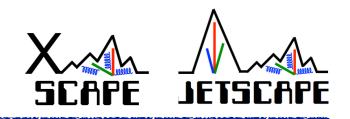
#### **Docker support**

One line of code to create environment with all software pre-reqs

For example: https://github.com/JETSCAPE/X-SCAPE/wiki/Doc.Installation.Docker.MacOS



## More Docker Containers ...



If you just want to use X-SCAPE/JETSCAPE as an out of the box event generator we provide fully compiled, ready to run Docker containers!



#### jetscape/xscape\_full ☆

By jetscape • Updated 3 months ago Image containing a full implementation of X-SCAPE.

Overview Tags		
xscape_full contains a full i. Comentation of X-SCAPE. The version numbers here are unrelated to X-SCAPE release versions. beta_v0.2		Docker Pull Command docker pull jetscape/xscape_full
Implements X-SCAPE	jetscape/jetscape_full ☆         By jetscape • Updated 3 months ago         Image containing a full implementation of JETSCAPE.         Image	Pulls 5
	Overview Tags	
	jetscape_full contains a full implementation of JETSCAPE. The version numbers here are unrelated to JETSCAPE release versions. beta_v0.2 • Implements JETSCAPE 3.5.4	Docker Pull Command docker pull jetscape_full

#### Joern Putschke, WSU

#### JETSCAPE 2023 Online School

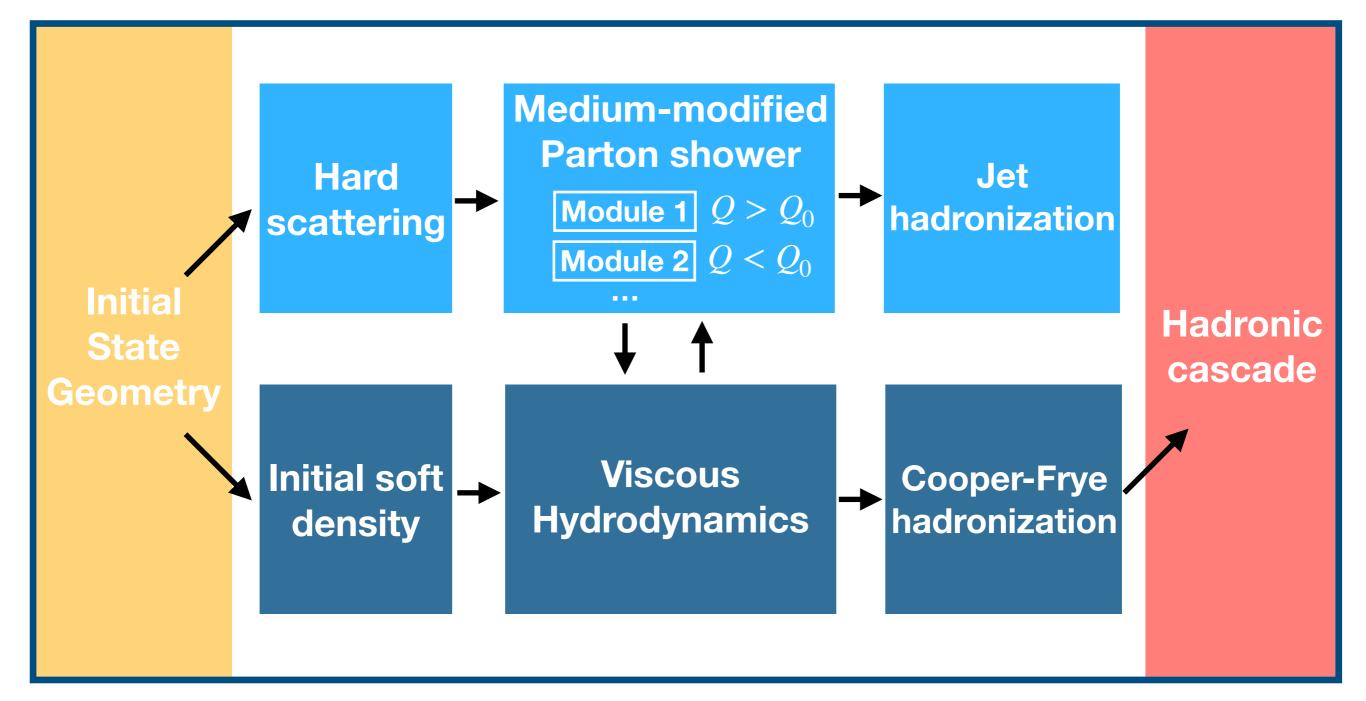
Pulls 10

## **JETSCAPE Event Generator**



#### JETSCAPE Manual: 1903.07706

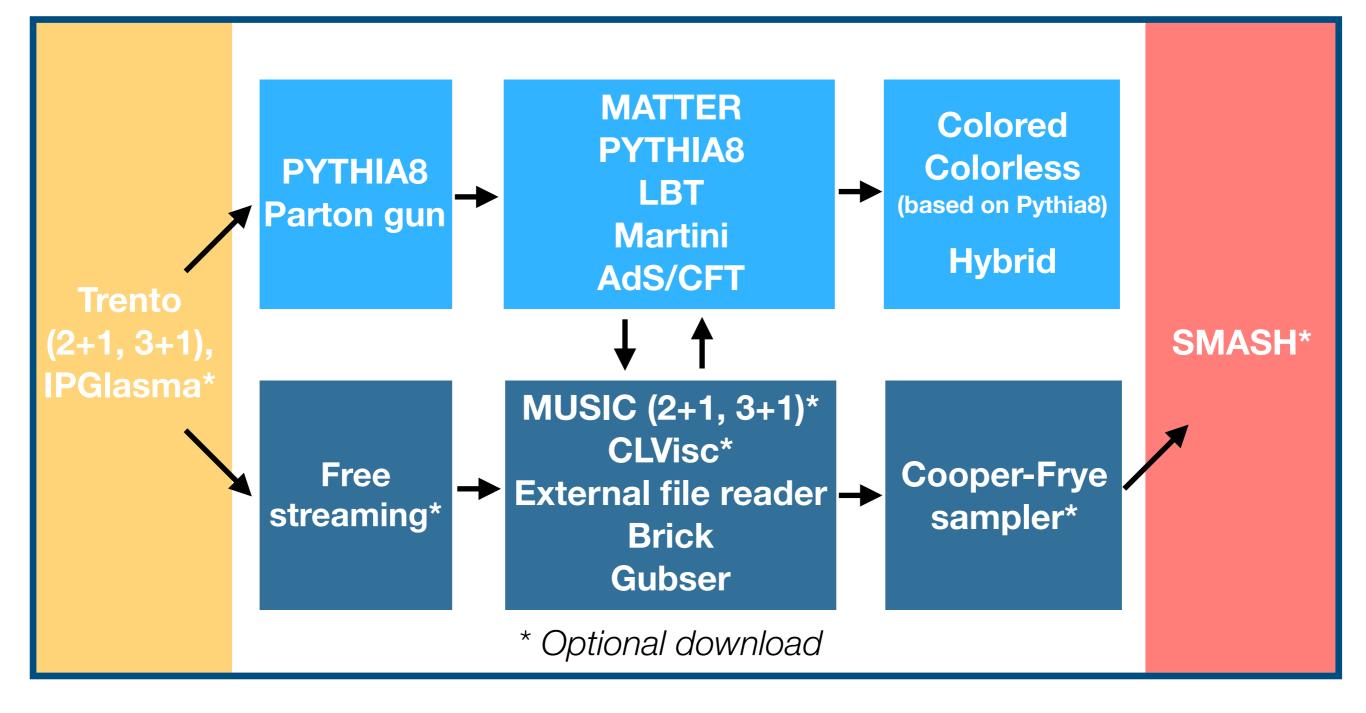
https://github.com/JETSCAPE/X-SCAPE





#### JETSCAPE Manual: 1903.07706

https://github.com/JETSCAPE/X-SCAPE





- 1. Install and build X-SCAPE (JETSCAPE)
- 2. Create a configuration file: config/jetscape\_user.xml List of which modules to run, and which model parameters to use See examples in: config/
- 3. Execute runJetscape

That's it!



### JETSCAPE is configured via two XML files

- Main XML file you don't modify this
  - Contains default values for every possible module and parameter
- User XML file you provide this
  - List of which modules to run, and which default parameter values to override

# **Configuring JETSCAPE**



#### Main XML file

you don't modify this

# A "database" of all possible modules and parameters

All possible initial state module parameters



# **Configuring JETSCAPE**



<jetscape> Set Writer <nEvents> 200 </nEvents> Set nEvents <!-- Jetscape Writer --> <JetScapeWriterAscii> on </JetScapeWriterAscii> **User XML file** <!-- Inital State Module --> <IS> you provide this <Trento use\_module="user\_defined"> </Trento> </IS> <!-- Hard Process --> <Hard> **Specify which** <PGun> </PGun> </Hard> modules to run <!-- Hydro Module --> Activate <Hydro> <MUSIC> </MUSIC> modules **Specify parameter** </Hydro> (in order) values (otherwise Override values <!--Eloss Modules --> <Eloss> taken from master) <Matter> <Q0> 2.0 </Q0> <qhat0> 5.0 </qhat0> </Matter> <AdSCFT> </AdSCFT> </Eloss> <!-- Jet Hadronization Module --> <JetHadronization> <name>colored</name> </JetHadronization> See examples in: config/ </jetscape>

JETSCAPE 2023 Online School



### There is one central executable\*: runJetscape.cc

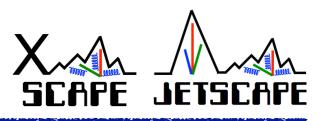
- Modules are automatically added according to User XML
- You don't ever need to re-compile this executable

### Pass your user configuration file as a command line argument:

./runJetscape /path/to/my/user\_config.xml

\* For integration in other frameworks/different usage you can of course also write your own executable see in GitHub ./examples/costum\_examples

## **JETSCAPE/X-SCAPE Output**



#### **JETSCAPE** output contains:

Final state hadrons Final state partons Full parton-shower history

#### You can produce JETSCAPE output in two formats\*:

#### Ascii

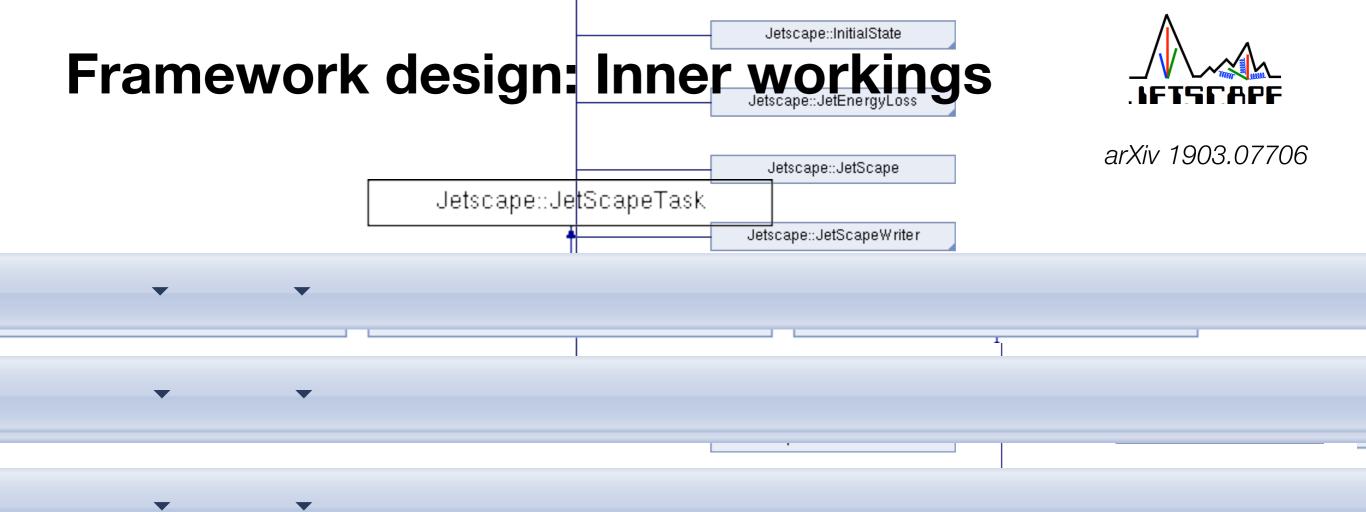
Custom JETSCAPE format Option to write (i) parton shower history, or (ii) only final-state particles Can also directly write gzipped ascii

#### HepMC3

Standard event format Ascii or ROOT format supported Compatible with Rivet \* You can easily write your own output class to tailor to

JETSCAPE 2023 Online School

your specific needs by inheriting from the JetScapeWriter

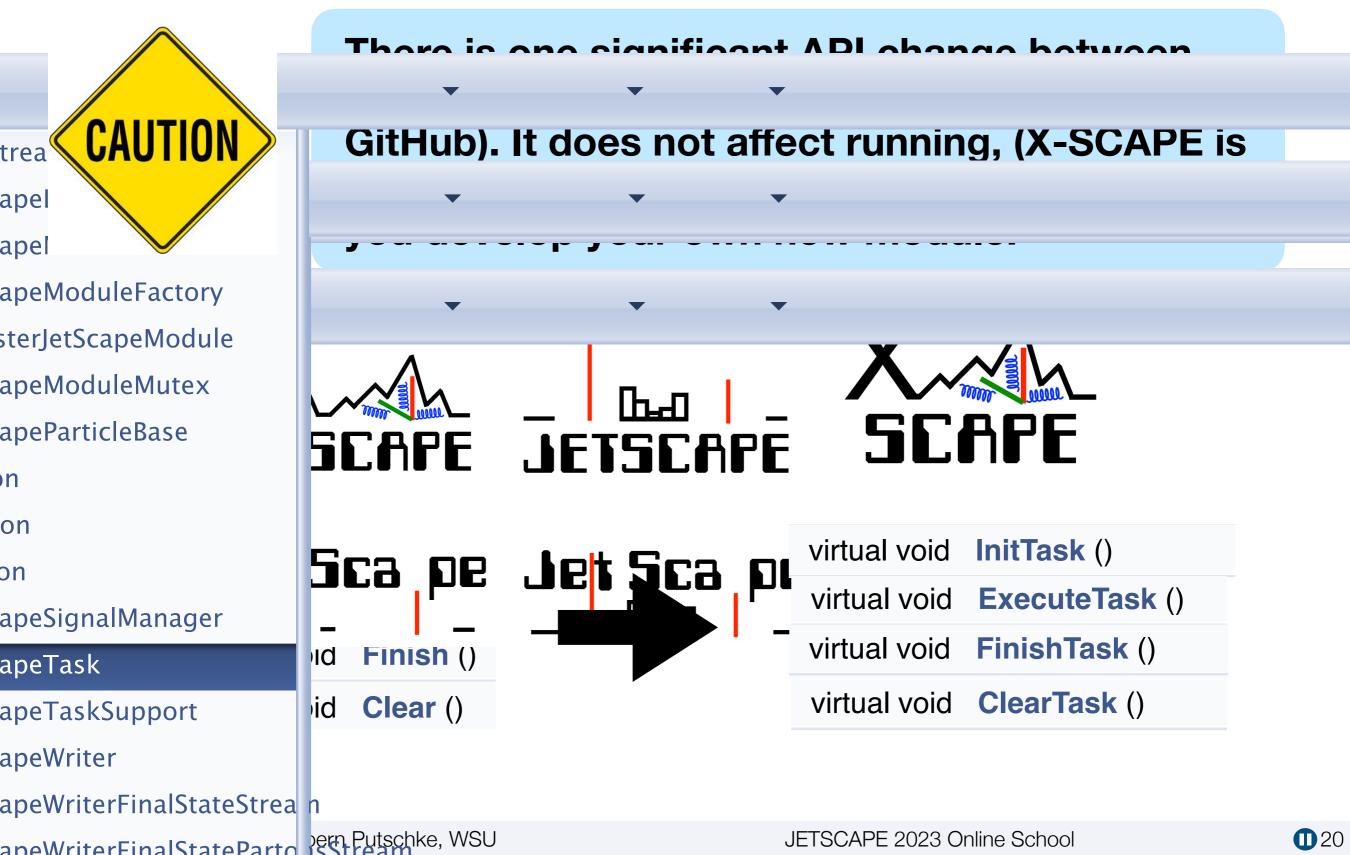


classes of JetScape lask	Jeiscapemaiuriocess
virtual void Init ()	lates an unitial State
The framework automatically calls	Jetscape::InitialState
standard functions of these modules:	Jetscape::JetEnergyLoss
virtual void ExecuteTasks ()	Jetscape::JetScape
virtual void E virtual void InitTask ()	
virtual void Ir	Jetscape::JetScapeWriter
virtual void ExecuteTask ()	
virtual void In virtual void FinishTask ()	Jetscape::PartonPrinter
virtual void C VIII VOID FIIIISIII ask ()	p
virtual void ClearTask ()	Jetscape::PreequilibriumDynamics
virtual void Fi	
virtual void FinishTasks ()	Jetscape::SoftParticlization
virtual void WriteTasks (weak_ptr< JetScapeWriter > w)	Jetso
<pre>virtual void WriteTask (weak_ptr&lt; JetScapeWriter &gt; w)</pre>	19

## Framework design: Inner workings



arXiv 1903.07706





arXiv 1903.07706

# The framework defines how different types of modules can interact with each other

For example: Jet energy loss module needs access to hydro info

#### This is implemented in a "signal-slot" paradigm\*:

Module 1	Module 2	Signal	Slot
JetEnergyLossManager	HardProcess	GetHardPartonList()	GetHardPartonList()
JetEnergyLoss	FluidDynamics	jetSignal()	UpdateEnergyDeposit()
JetEnergyLoss	FluidDynamics	edensitySignal()	GetEnergyDensity()
JetEnergyLoss	FluidDynamics	GetHydroCellSignal()	GetHydroCell()
JetEnergyLoss	JetEnergyLoss	SentInPartons()	DoEnergyLoss()
Hadronization	Hadronization	TransformPartons()	DoHadronization()
HadronizationManager	HardProcess	GetHadronList()	GetHadronList()
HadronizationManager	JetEnergyLoss	GetFinalPartonList()	SendFinalStatePartons()

Table 3: The list of all connection methods between JETSCAPE modules provide by the JetScapeSignalManager. \* Introduced by the QT framework

Joern Putschke, WSU

JETSCAPE 2023 Online School

# Framework design: Inner workings



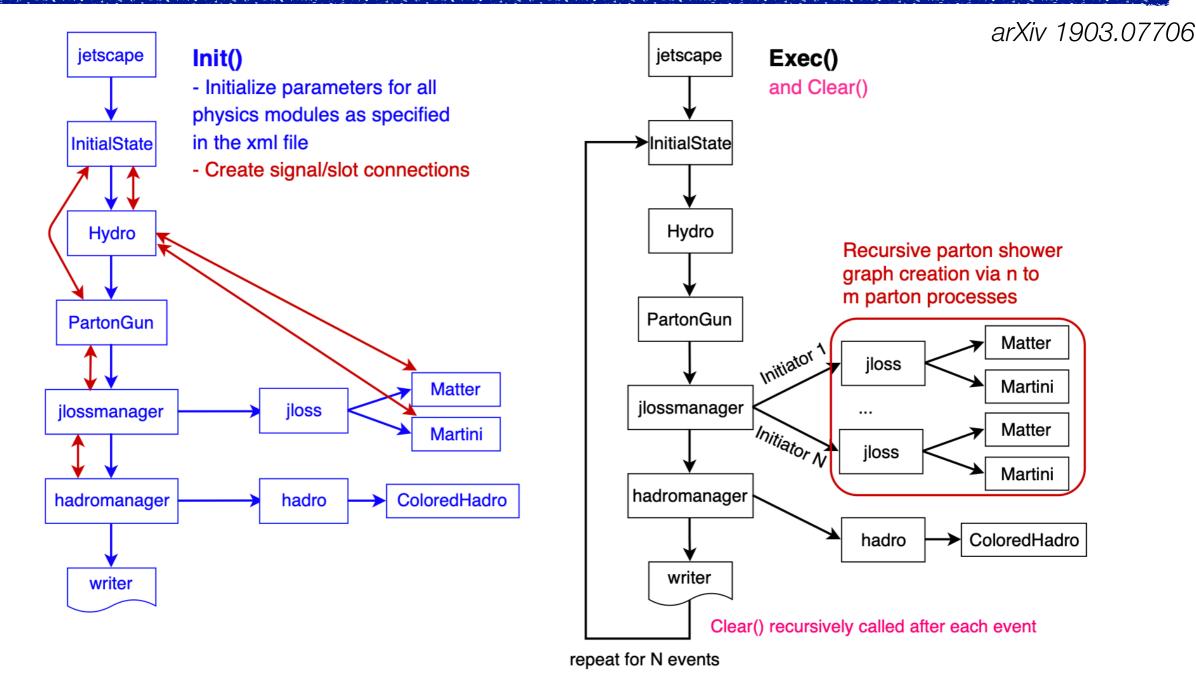


Figure 4: Example workflow of the Init() (left side) and Exec() (and Clear()) (right side) phase of the task based JETSCAPE framework (the not extensively used Finish() phase is omitted). One should be aware that the created signal/slot connections in the Init() phase are of course present and utilized in the Exec() phase, but are not show in the figure for simplicity.

JETSCAPE 2023 Online School

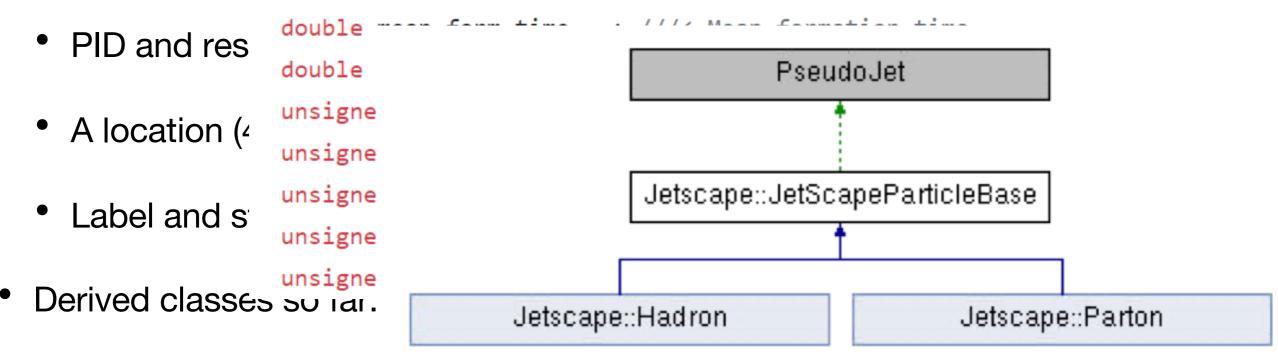
# **Data structures**

SCAPE JETSCAPE

arXiv 1903.07706

Class JetScapeParticleBase

- The base class for all the JETSCAPE particles
- Privately inherits from FastJet PseudoJet and has
   protected :

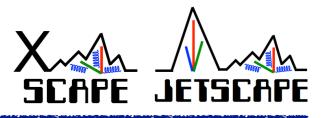


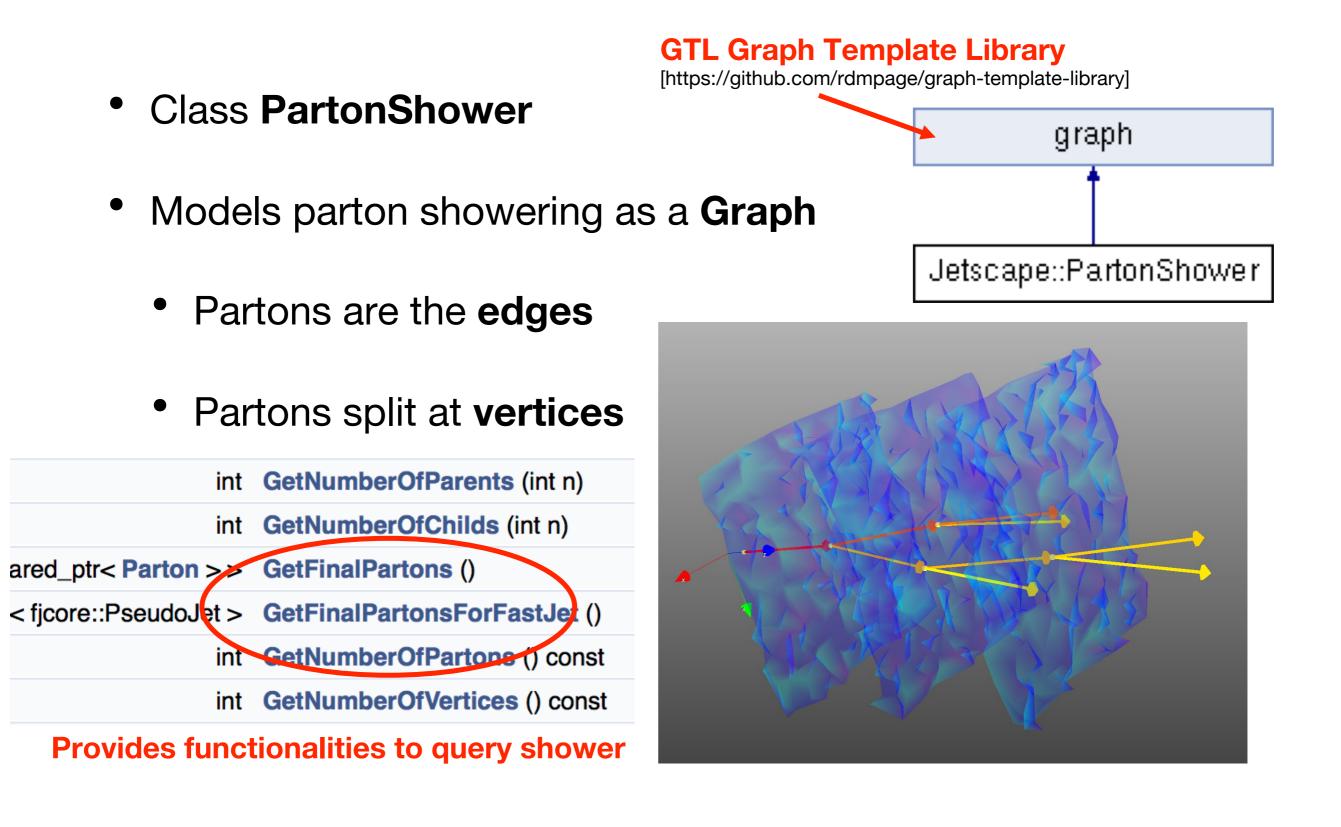
Parton and Hadron

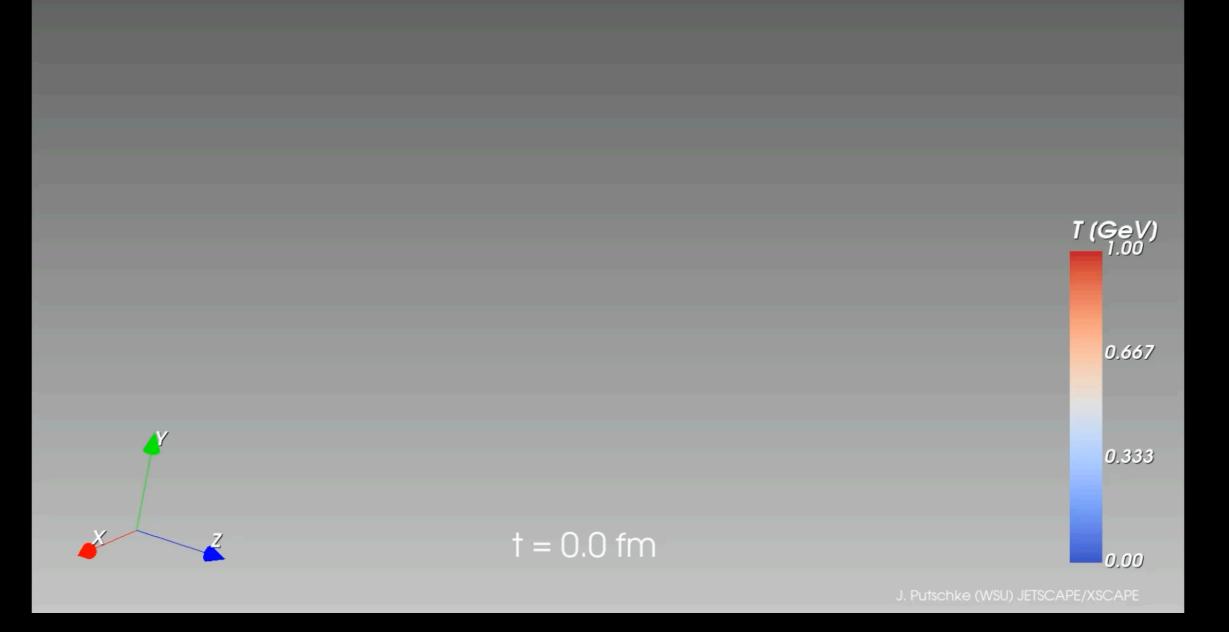
Parton (int label, int id, int stat, const FourVector& p, const FourVector& x);
Parton (int label, int id, int stat, double pt, double eta, double phi, double e, double\* x=0);
...

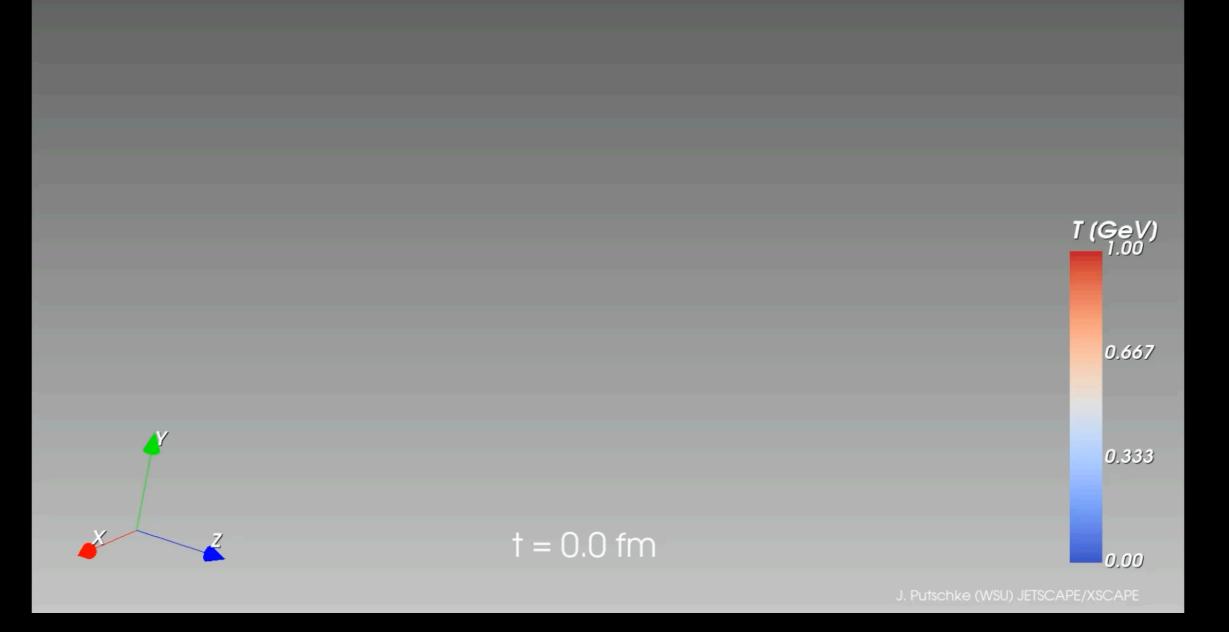
In addition: Photon class (inherits from Parton)

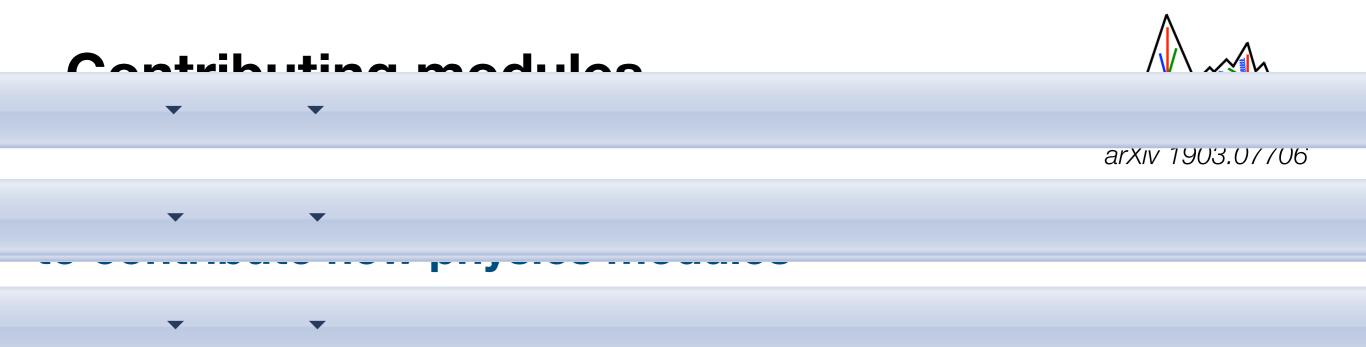
## **Data structures**











## To contribute modules, just need to interface to JETSCAPE:

## Implement appropriate standard functions:

virtual void InitTask ()

virtual void ExecuteTask ()

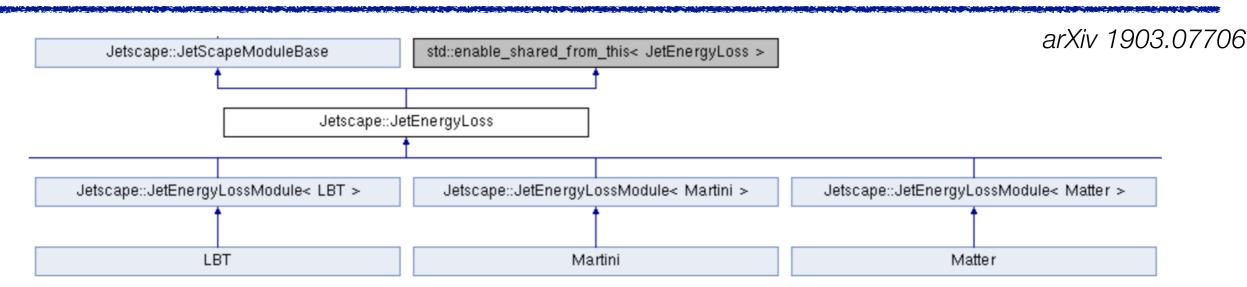
virtual void FinishTask ()

virtual void ClearTask ()

Use appropriate signal/slot info to interact with other modules

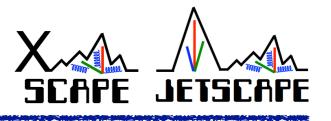
## See existing modules for examples

## **Example: Jet energy loss**



- User's code must be a subclass of **JetEnergyLossModule**
- User's code must override init() method for initializations
- User's code must override **DoEnergyLoss()** method
  - The actual energy loss calculations happen in this method

**Note:** Jet energy loss modules are "special" in that DoEnergyLoss() is called by the framework **per-parton**. Most modules are called **per-event** with Exec()



arXiv 1903.07706

# An XML singleton class is provided to allow easy initialization of your module parameters from the XML files

- JetScapeXML provides functionality to first examine the User file for a given parameter, and if it is not found, it takes the value from the Master file.
- To init a parameter, call GetElementDouble({"Eloss", "Martini", "x"})
  - No need to keep track of XML elements in modules! Just call the function!
  - Similar functions *GetElementText*, *GetElementInt*, *GetElement*
- An optional second argument in these functions allows the parameter to be optional in the XML file (by default, a parameter is required to be present or else the program will crash when it is not found).

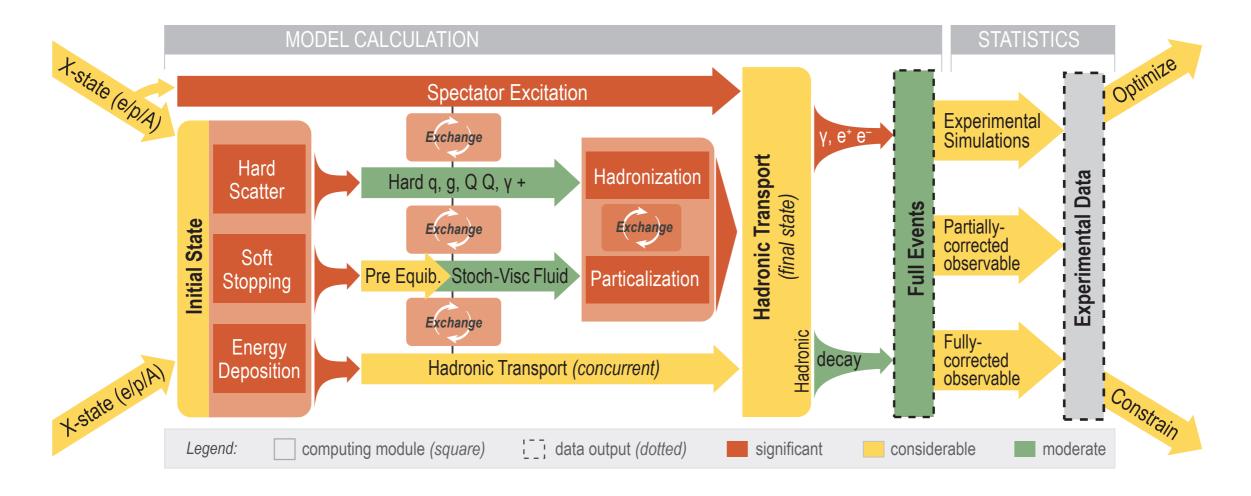




Remark: X-SCAPE 1.0 is not fully steered via XML, you have use a separate executable (see documentation for details). Will be changed in upcoming releases.

## **X-SCAPE: Extended Physics Scope**



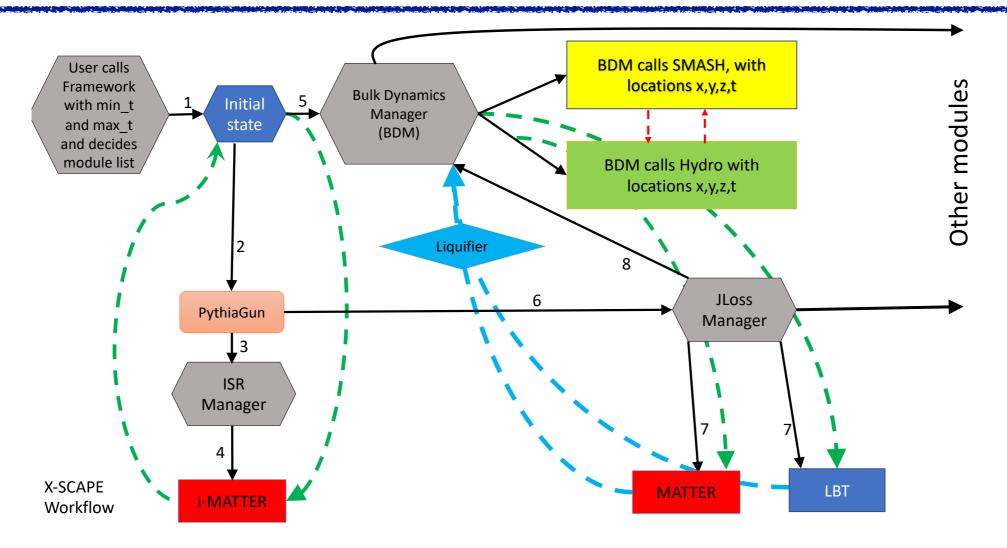


XSCAPE framework goal: To provide a *decentralized and synchronized* framework, which will allow any user to attach his/her own modules and reorganize the flow of data between the modules with the goal to simulate:

To simulate *p*-*A* and *p*-*p* collisions at arbitrary multiplicity (X-SCAPE 1.0)
 Any aspect of *A*-*A* collisions from FAIR to top LHC energy (X-SCAPE 2.0)
 To study *e*+*e*-and certain aspects of *e*-*A* collisions (X-SCAPE 3.0)

# **X-SCAPE: Extended Physics Scope**



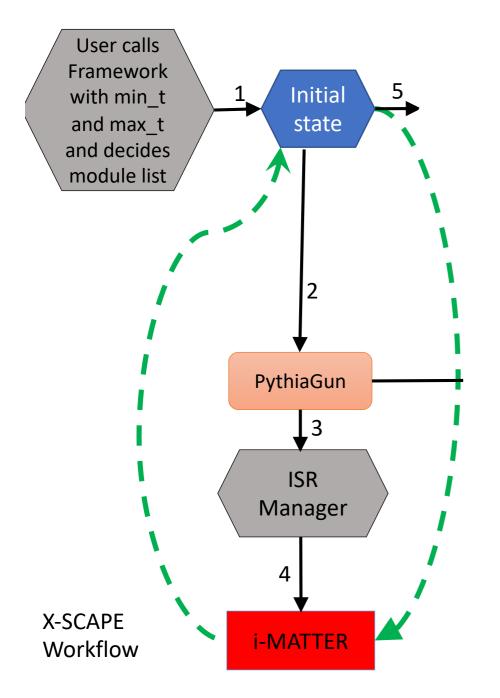


XSCAPE framework goal: To provide a *decentralized and synchronized* framework, which will allow any user to attach his/her own modules and reorganize the flow of data between the modules with the goal to simulate:

To simulate *p*-*A* and *p*-*p* collisions at arbitrary multiplicity (X-SCAPE 1.0)
 Any aspect of *A*-*A* collisions from FAIR to top LHC energy (X-SCAPE 2.0)

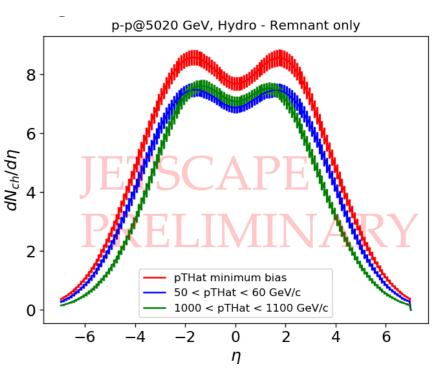
# **X-SCAPE 1.0: Small Systems**





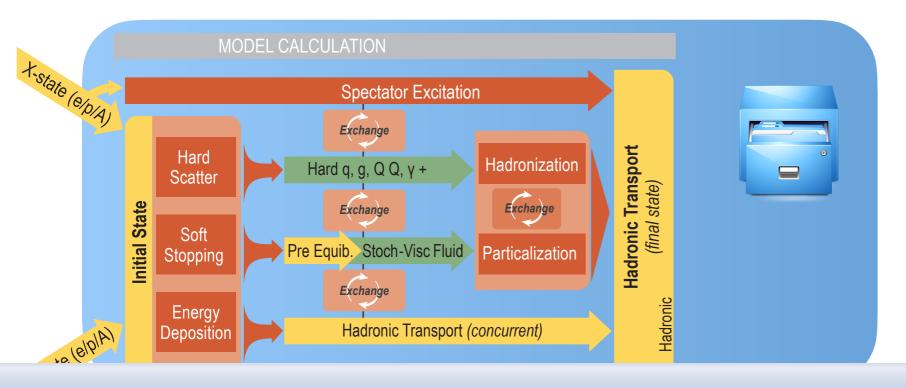
Provide new **ISR Manager** module, inherited from the JetEnergyLossManager, but evolves "backward" in time\* to simulate the initial state radiation and allows exchange/interaction with the InitialState module (3dGlauber for example).

Hard energy removed from nucleons, not available for hydro evolution! (Hard Probes 2023)



\*<u>Remark</u>: For now ISR Manager and backward time evolution is utilized for simplicity on a per-event basis (clock and per time-step evolution is working, but not utilized as default)

# Simplified/more flexible data exchange



"Database" query approach using any(variant) datatype via **QueryHistory instance** 



Implement GetHistory() in Jetscape Module(s). Can hold "any" datatype, in particular allows non framework datatypes\*!

\*Caveat: Since an any datatype has to explicitly be casted, this new flexible data exchange might break the stringent API and only framework datatype approach of "every module works with every other module" of JETSCAPE. Might change in the future, using variant or might be defunct.

LA Searc

## Simplified/more flexible data exchange

nerator neratorDefat t 8 arameterFile ynamics

#### Jetscape::QueryHistory Class Reference

#include <QueryHistory.h>

Public Member Functions

void	AddMainTask (std::shared_ptr< JetScapeTask > m_main_task)
void	UpdateTaskMap ()
void	PrintTasks ()
void	PrintTaskMap ()
d::unordered_multimap< std::string, std::weak_ptr< <b>JetScapeTask</b> >>	GetTaskMap ()
any	GetHistoryFromModule (string mName)
vector< any >	GetHistoryFromModules (string mName)

•••

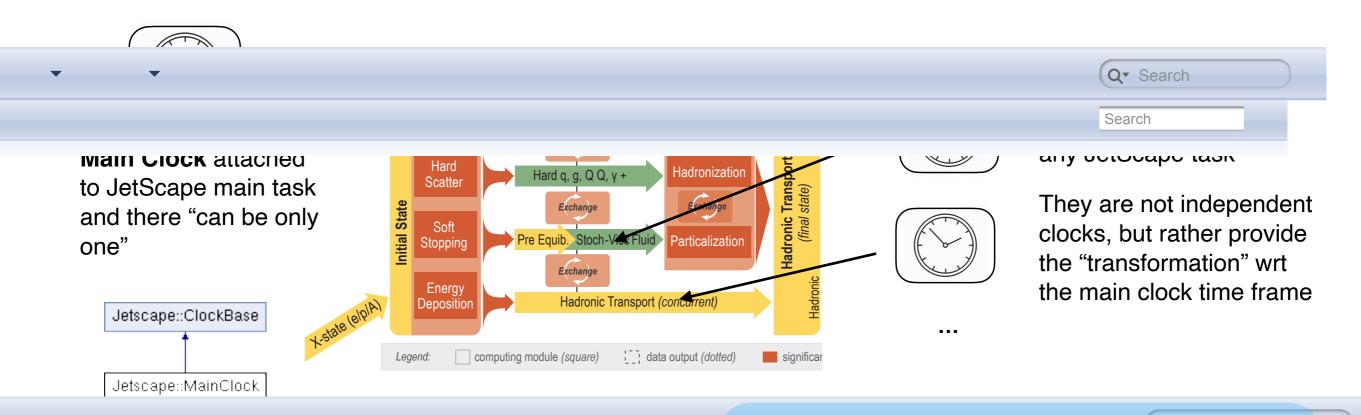
QueryHistory Instance queries tasks via string identifier and retrieves information from GetHistory() if implemented.

Generated by OOXYGEN 1.9.1 Querynistory:::Instance()--/ GetHistoryFromModules ("JetEnergyLoss");

Q- Search

# Clock(s) in X-SCAPE ...





JetScapeModuleBase ()

JetScapeModuleBase (string m\_name)

bool IsTimeStepped () const

Returns whether the module evolves in time steps. More...

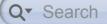
void SetTimeStepped (bool m\_time\_stepped)

Sets whether the module evolves in time steps. More...

<u>Remark:</u> Has to be set explicitly to true, default is false, so per event "JETSCAPE" like execution.

If a main clock is attached to the main task, physics modules can be executed (no module clock needs to be provided, by default main clock will be used) on a per time-step basis! In general, one can mix per event and per timestep, if it makes sense from a physics perspective.

•	• •	Q• Search
eam <b>TLLUVI</b> m mFilter		SEAPE
	ScapeModuleBase.h>	
Inheritance diagra	m for Jetscape::JetScapeModuleBase: Jetscape::JetScapeTask sigslot::has_slots< sigslot::	
• •	•	Q Search
Public Member Fund	ctions	
a	TimeModule ()	auto mClock =
a	TimeModule (double t1, double t2)	<pre>make_shared<mainclock>("SpaceTime",</mainclock></pre>
virtual	~TimeModule ()	-0.1,0.1,0.1);
n void	ClockInfo ()	auto mMilneClock =
void	AddModuleClock (shared_ptr< ModuleClock > m_mClock)	make shared <milneclock>();</milneclock>
shared_ptr< ModuleClock >	0	mMilneClock->setEtaMax(5.0);
	AddMainClock (shared_ptr< MainClock > m_mainClock)	
	UseModuleClock ()	auto jetscape =
	GetModuleCurrentTime () GetModuleDeltaT ()	make_shared <jetscaperate) \$="" 1.9.1<="" doxygen="" td=""></jetscaperate)>
	IsValidModuleTime ()	jetscape->AddMainClock(mClock);
	SetTimeRange (double t1, double t2)	auto hydro = make shared <brick> ();</brick>
	GetTStart () const	hydro->SetTimeRange(0.6,10);
const double	GetTEnd () const	hydro->AddModuleClock(mMilneClock);
		hydro->SetTimeStepped(true);



\/

JetScapeModuleBase ()

#### JetScapeModuleBase (string m\_name)

bool IsTimeStepped () const Returns whether the module evolves in time steps. More...

void **SetTimeStepped** (bool m\_time\_stepped) Sets whether the module evolves in time steps. More...

virtual void CalculateTime ()

virtual void	CalculateTimeTask ()
virtual void	ExecTime ()
virtual void	ExecTimeTasks ()
virtual void	ExecTimeTask ()
virtual void	InitPerEvent ()
virtual void	InitPerEventTasks ()
virtual void	FinishPerEvent ()
virtual void	FinishPerEventTasks ()

JetScapeModuleBase provides an additional per time-step workflow:

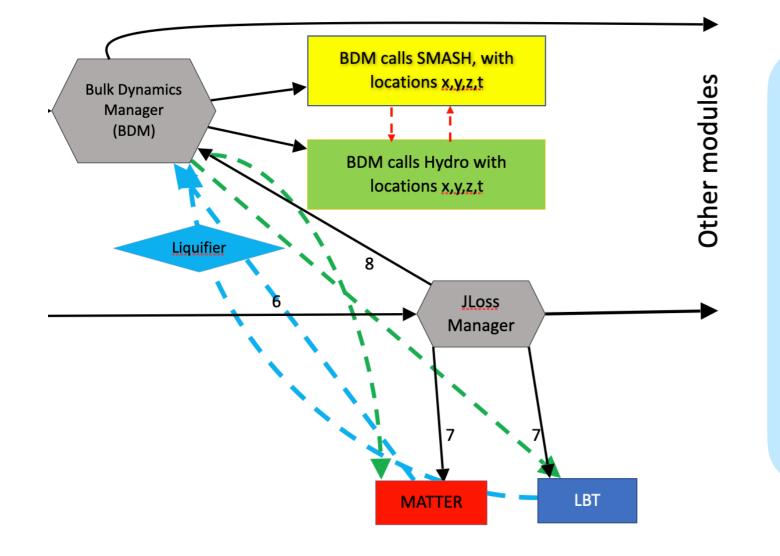
- CalculateTime() phase: Module(s) simulate the next timestep. No communication between modules -> can be trivially multithreaded if needed.
- 2) ExecTime() phase: by doxygen 1.9.1 Communication/data exchange etc. between modules needed before next time-step

<u>Remark:</u> If you want to develop modules which can be executed per time-step you have to provide these functions, analogous to InitTask(), ExecTask(),... in the JETSCAPE workflow.

Generated by OOXVOE

**D**36



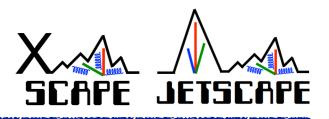


#### BulkDynamicsManager (BDM):

Organizes/allows concurrent running of multiple QCD bulk media implementations!

Initially for X-SCAPE 2.0 (release expected end of this year) hydro (MUSIC) and hadron cascade (SMASH), focus on low beam energy AA collisions!

First proof-of-principle implementation of the BDM and other example/test programs utilizing the new X-SCAPE per time-step workflow can be found in the custom example directory!



### JETSCAPE/X-SCAPE is a framework for general-purpose e-A, p/d-A and A-A event generators

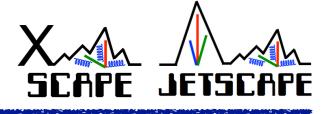
• Modular, extensible — please contribute modules!

### **JETSCAPE/X-SCAPE** is a tool for the community

- To enable well-controlled event generator comparisons
- As a testbed for theoretical and experimental development

## JETSCAPE (X-SCAPE) has been successfully used and tested in large scale simulation efforts

# Remarks on large scale simulations X



JETSCAPE has used **tens of millions of core-hours running simulations** for Bayesian analyses (covered next week) which are especially computationally expensive. When you run simulations at scale, here are some details to consider:

- Containers simplify deployment when running simulations at scale
- Utilize **singularity containers** (see GitHub installation instructions)
  - Most High Performance Computing (HPC) sites will not allow you to use docker containers
  - You can directly convert the docker container into a format suitable for singularity
- Make sure you build your container in a reproducible way by explicating setting the versions of dependencies
  - If you take the most recent version, it may change next time you build the container
  - That can change your physics!
- Be aware of HPC facility architecture, capabilities, requirements, and best practices
- Particularly watch out for file I/O limits; for example, reading pre-computed hydro profiles for use in jet energy loss calculations can be a high IO activity
- Write output files to the **temporary storage** of the computing node, and then copy only the files you need back to permanent storage; consider calculating observables directly from outputs
- **Optimize** for the type of simulation that you are running:
  - Hydro utilizes multi-core capabilities → Request many cores on a single node
  - Jet energy loss uses a core at time (massively parallel)  $\rightarrow$  Cores can be from any node







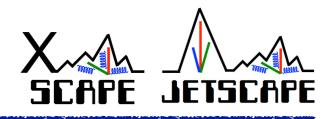


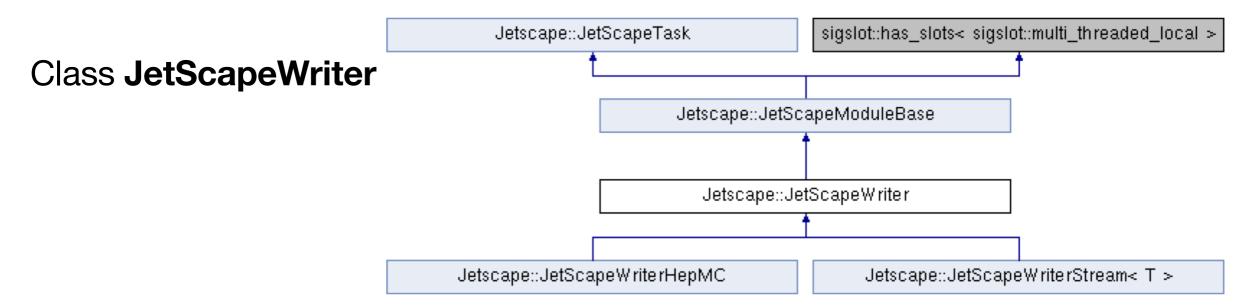
# Backup

Joern Putschke, WSU

JETSCAPE 2023 Online School

41





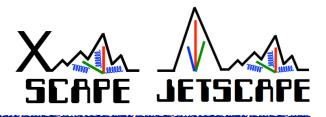
Subclass of JetScapeModuleBase

• Can be attached as a task

Derived classes so far:

- HepMC writer
- ASCII writer

	E	ach task overrides its	•
virtual void	FinishTask ()	own write method	
virtual void	FinishTasks ()		
virtual void	WriteTasks (weak_	ptr< JetScapeWriter > w)	
virtual void	WriteTask (weak_p	otr< JetScapeWriter > w)	
virtual void	CollectHeader (we	ak_ptr< <b>JetScapeWriter</b> > w)	
virtual void	CollectHeaders (w	eak_ptr< <b>JetScapeWriter</b> > w)	



#### Class JetScapeReader

Base class for reading JETSCAPE output files

