Software Design Document: GPU N-Body Integration Toolkit

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1 Introduction

1.1 Purpose

This document serves as the system design for the GPUnit framework to control AMUSE experiments as set forth in the Software Requirements Specification. AMUSE (Astrophysical Multipurpose Software Environment) is a software package and set of legacy codes for performing astrophysics simulations. For more details on the purpose and use cases of AMUSE, please refer to our SRS. The goal of this document is to provide details guiding the construction of the framework, as well as to provide a reference to the framework's architecture. It contains specifications for the objects used by the system and our initial reference implementation plans.

1.2 Scope

This document will describe the implementation for our framework, covering the network layer, the user interface and the core python command line scripts. It will cover user interface support classes as they will need to be coded, however the actual UI components such as windows and widgets will not be described. Code and objects for these items are generated as part of the Qt Creator¹ GUI development kit. As such, the code is not intended to be human-readable and is subject to change between Qt versions. Our SRS document contains the reference prototype which will serve as the design for the GUI widgets. The data models including experiment file layouts and network packet details will also be covered.

1.3 Glossary

For terms not in this glossary, please refer to the SRS.

Cluster A group of networked computing nodes available to perform some task.

Computer Node A computer that is a member of a cluster.

IPC Channel Any object or memory space used for Inter-Process Communication (IPC). Examples include UNIX Pipes, BSD/Winsock Sockets and UNIX Shared Memory (SHM).

Node Health Statistics Information about the current state of a node including properties such as CPU usage and memory usage.

 $^{^{1}} http://qt.nokia.com/products/developer-tools/\\$

2 Architecture

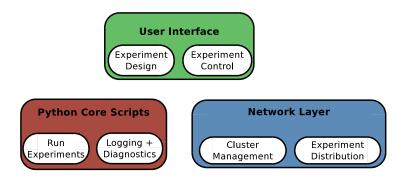


Figure 2.1: Architecture Diagram

3 Graphical User Interface

3.1 Overview

The user interface will allow the user to create and manage experiments as described in the SRS. Much of the interface code is generated from the GUI development tools, however there are some support classes required for the GUI to interact with the network and the command line tools.

3.2 Network Interaction

The network interaction classes allow the UI to send and receive messages through a control instance (Section 6.2.1). The control instance can be either running locally or on a remote machine. The UI uses this link to query the cluster for status updates and control running experiments.

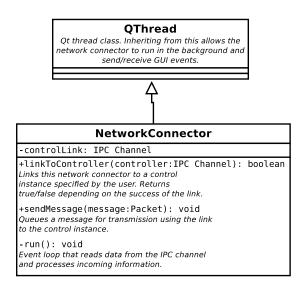


Figure 3.1: GUI Network Connection Class

3.3 Node Management

Nodes in the cluster, detected through the network connector, may be viewed in the node view window. (Satisfies requirements 2.8.1.X)

From the node window, the user can assign experiments to individual nodes. (Satisfies requirement 2.8.2.1)

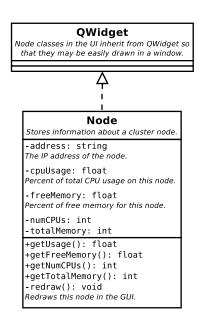


Figure 3.2: Node Class

4 Experiment Components

Experiment

4.1 Experiment Object Model

```
An experiment holds all used particles, modules,
                                                                     Sets the name of the experiment to the given
                logging tools, diagnostics, and initial
                    conditions for a simulation.
                                                                     +getName(): string
             It is able to evolve the state of the particle
                                                                     Returns the name of the experiment.
          system by the supplied timestep and retrieve the
            current state of the system. By default, this
                                                                     +setTimeStep(timeStep:UnitType): void
            evolution includes AMUSE's built-in stopping
                                                                     Sets the timestep to use in the simulation.
                           conditions.
          The supplied diagnostics gather information from
                                                                     +getTimeStep(): UnitType
           the simulation, and the supplied loggers report
                                                                     Returns the currently set timestep for the
               on the status of the system during the
                                                                     simulation.
                           simulation.
                                                                     +disableStopConditions(): void
          An experiment is also able to read from and write
                                                                     Disables stopping conditions by setting
               to XML files for persistence and reuse.
                                                                     stopisEnabled to false.
name: string
                                                                      enableStopConditions(): void
The name of the experiment
                                                                     Enables stopping conditions by setting
-timeStep: UnitType
                                                                     stopisEnabled to true.
The amount of time between each snapshot of the
                                                                      ⊦addModule(module:Module): void
particle system.
                                                                     Adds a module to the experiment.
-stopIsEnabled: boolean = true
                                                                     +removeModule(module:Module): void
True if stopping conditions are enabled.
                                                                     Removes the given module from the experiment
-modules: List∢Module>
                                                                      -addModules(modules:List<Module>): void
A list of modules used in the experiment.
                                                                     Adds the given list of modules to the experiment.
-particles: List<Particle>
                                                                     +addParticle(body:Particle): void
The list of particles to use in the experiment.
-diagnostics: List<Diagnostic>
                                                                     +removeParticle(body:Particle): void
The list of diagnostics to use in this
                                                                     Removes the given particle from the experiment.
experiment.
                                                                     +addParticles(bodies:List<Particle>): void
-loggers: List<Logger>
                                                                     Adds the given particles to the experiment.
This list of logging tools to use in the
experiment.
                                                                      ⊦addDiagnostic(diag:Diagnostic): void
                                                                     Adds the given diagnostic to the experiment.
+writeXMLFile(fileName:string=name): void
Writes the experiment description to the
                                                                     +removeDiagnostic(diag:Diagnostic): void
designated file in XML format
                                                                      The diagnostic to remove from the experiment
+<<static>> loadXMLFile(fileName:string): Experiment
                                                                      +addDiagnostics(diags:List<Diagnostic>): void
Loads experiment attributes from the given XML
                                                                     Adds the given list of diagnostics to the
+getCurrentState(): List<Particle>
                                                                     +addLogger(logger:Logger): void
Retrieves the list of particles to read their
                                                                     Adds the given logger to the experiment.
respective current states.
                                                                     +removeLogger(logger:Logger): void
+evolveState(): void
                                                                     Removes the given logger from the experiment.
Evolves/Updates the current state of the
                                                                      +addLoggers(loggers:List<Logger>): void
particles in the experiment by the experiment's timestep.
                                                                     Adds the given list of loggers to the experiment.
```

+setName(name:string): void

Figure 4.1: Experiment Class Diagram

4.1.1 Experiment Class

An instance of the Experiment class represents a single AMUSE experiment. It holds all particles (Satisfies requirement 2.3.3), modules, logging tools, diagnostics, and initial conditions for a simulation. These are described in more detail below. The experiment class can be viewed in Figure 4.1.

4.1.1.1 Experiment Attributes Experiments have the following attributes. The type UnitType is defined later in this document.

Name	Туре	Description	
name	string	The name of the experiment.	
timeStep	UnitType	The amount of time between	
		each snapshot of the simulation.	
stoplsEnabled	boolean	Whether or not stopping	
		conditions are enabled.	
modules List <module></module>		The list of Modules used in the	
		experiment.	
particles List <particle></particle>		The list of Particles to use in the	
		experiment.	
diagnostics	List < Diagnostic >	The list of Diagnostics to use in	
		the experiment.	
loggers List <logger></logger>		The list of Loggers to use in the	
		experiment	

4.1.1.2 Experiment Operations

void writeXMLFile(string		static Experiment loadXMLFile(string fileName)	
	eName)	Input	A string containing the filename to load the
Input	A string containing the filename to write the		Experiment XML from.
	Experiment XML file to.		The Experiment specified by the XML
Output Description	Output (none) Description Writes the Experiment		file.
in XML format to the specified filename.		Description	Recreates an Experiment from its XML specification.

List <	<particle></particle>		
getCurrentState()		VOI	id evolveState()
Input	(none)	Input	(none)
Output	The list of Particles in	Output	(none)
	the Experiment	Description	Evolves/Updates the
Description	Returns the list of		current state of the
	Particles in the		particles in the
	simulation with their		Experiment by the
	updated attributes to		Experiment's timeStep.
	read their current states.		

void setNa	me(string name)		
Input	A string containing the	string getName()	
•	updated Experiment	Input	(none)
	name.	Output	A string containing the
Output	(none)		name of the Experiment.
Description	Updates the	Description	Returns the name of the
	Experiment's name to		Experiment.
	the given parameter		
	neStep(UnitType		
tir	neStep)	Unit	ts getTimeStep()
Input	A UnitType containing	Input	(none)
	the updated Experiment	Output	A UnitType containing
	timeStep.		the Experiment
Output	(none)		timeStep.
Description	Updates the	Description	Returns the timeStep of
	Experiment's timeStep		the Experiment.
	to the given parameter.		
void disableStopConditions()		void enableStopConditions()	
Input	(none)	Input	(none)
Output	(none)	Output	(none)
Description	Disables the	Description	Enables the
	Experiment's stopping		Experiment's stopping
	conditions.		conditions.
	Module(Module	void removeModule(Module module)	
m	nodule)	Input	A Module to remove
Input	A Module to add to the		from the Experiment.
	Experiment.	Output	(none)
Output	(none)	Description	Removes the given
Description	Adds the given Module		Module from the
	to the Experiment.		Experiment
	void addModules(List <module></module>		icle(Particle body)
m	modules)		A Particle to add to the
Input	A list of Modules to add	Input	Experiment.
	to the Experiment.	Output	(none)
Output	(none)	Description	Adds the given Particle
Description	Adds the given Modules	Description	to the Experiment.
	to the Experiment.		to the Experiment.

void addParti	cles(List <particle></particle>	void removeParticle(Particle body)	
Ŀ	odies)	Input	A Particle to remove
Input	A list of Particles to add		from the Experiment.
	to the Experiment.	Output	(none)
Output	(none)	Description	Removes the given
Description	Adds the given Particles		Particle from the
	to the Experiment.		Experiment.
void addDiag	gnostic(Diagnostic	void a	ddDiagnos-
	diag)		<diagnostic></diagnostic>
Input	A Diagnostic to add to		diags)
_	the Experiment.	Input	A list of Diagnostics to
Output	(none)		add to the Experiment.
Description	Adds the given	Output	(none)
	Diagnostic to the	Description	Adds the given
	Experiment Satisfies		Diagnostics to the
	requirement $2.6.3.\{1,2\}$.		Experiment.
void removeD	void removeDiagnostic(Diagnostic diag)		ger(Logger logger)
Input	A Diagnostic to remove	Input	A Logger to add to the
Input	from the Experiment		Experiment
Output	(none)	Output	(none)
Description	Removes the given	Description	Adds the given Logger
Beschiption	Diagnostic from the		to the Experiment
	Experiment.		Satisfies requirement
	Experiment.		2.7.1.
void addLogs	gers(List <logger></logger>	void removeLogger(Logger logger)	
loggers)		Input	A Logger to remove
Input A list of Loggers to add			from the Experiment.
to the Experiment.		Output Description	(none)
Output	·		Removes the given
Description	- ,		Logger from the
2 cociiption	to the Experiment.		Experiment. Satisfies
	to the Experiment.		requirement 2.7.2.

4.2 Particles

Particles are the elements that are being updated and the experiment is being run on. These particles can be anything as little as atoms to as large as star clusters. They are made up of mass, position, and velocity. (Satisfies requirements 2.3.1, 2.3.2)

4.2.1 Particle Class

Particle
-mass: Parameter -velocity: Parameter -position: Parameter
-position: Parameter +getVelocity(): Parameter +setVelocity(v:List <double>,unit:Unit): boolean</double>
<pre>+getPosition(): Parameter +setPosition(pos:List<double>,unit:Unit): bool +getMass(): Parameter</double></pre>
+setMass(mass:double,unit:Unit): bool

Figure 4.2: Particle Class Diagram

Particle class will be instantiated and used for storage of particle type items on the UI of GPUnit. The Particle class in AMUSE will be used in the CLT. The particle class will be used primarily for data storage for experiment creation.

4.2.1.1 Particle Attributes

Name Type		Description		
mass	Parameter	The current mass of the particle.		
		Will have units.		
velocity	Parameter	The current mass of the particle.		
		Will have units.		
position	Parameter	The current position of the		
		particle. Will have units.		

4.2.1.2 Particle Methods

Parameter getMass()		bool setMass(double mass, Unit unit)	
Input (none)		Input	The new value of the mass and the unit it is
Output	A parameter with the value and units of the current mass.	Output	in. Returns true if the mass
Description	Gets the current value of the mass.	Description	is successfully set. Sets the mass of the particle.

L_			
		bool setVelocity(List <double> v, Unit unit)</double>	
Parameter getVelocity()		Input	The new vector value of
Input	(none)		the velocity and the unit
Output	A parameter with the		it is in.
	value and units of the	Output	Returns true if the
	current velocity.		velocity is successfully
Description	Gets the current value of		set.
	the velocity.	Description	Sets the velocity of the
			particle.

		bool setPosition(List <double> pos, Unit unit)</double>	
Parameter getPosition()		Input	The new vector value of
Input	(none)		the position and the unit
Output	A parameter with the		it is in.
	value and units of the	Output	Returns true if the
	current position.		position is successfully
Description	Gets the current value of		set.
	the position.	Description	Sets the position of the
			particle.

4.3 Modules

This section defines an object model for the representation of and interaction with AMUSE modules, including several ancillary types utilized by the module implementation.

4.3.1 Module Class

Module
-name: string
-description: string
-domain: AstrophysicalDomain
-codeName: string
-codeLocation: string
-isParallel: boolean
-stoppingConditions: StoppingConditions
-parameters: List <parameter></parameter>
+getName(): string
+setName(name:string): void
+getDescription(): string
+setDescription(description:string): void
+getAstrophysicalDomain(): AstrophysicalDomain
+setAstrophysicalDomain(domain:AstrophysicalDomain): void
+getCodeName(): string
+setCodeName(codeName:string): void
+getCodeLocation(): string
+setCodeLocation(codeLocation:string): void
+getParallelism(): boolean
+setParallelism(isParallel:boolean): void
+getStoppingConditions(): StoppingConditions
+setStoppingConditions(conds:StoppingConditions): void
+getParameters(): List <parameter></parameter>
+setParameters(parameters:List <parameter>): void</parameter>
+addParameter(p:Parameter): void
+removeParameter(p:Parameter): boolean
+toXml(): string
+fromXml(element:string): Module

Figure 4.4: Module class diagram

An instance of the Module class represents a particular AMUSE module, providing an interface between GPUnit and the AMUSE code. The members of the Module class are used by GPUnit to properly locate and initialize an AMUSE module, as well as display a module's details and configuration to the user in the graphical interface. (Satisfies requirements 2.2.1, 2.2.2, 2.2.3, 2.2.4, 2.2.5)

4.3.1.1 Module Attributes

3.1.1 Module Attri Name	Туре	Description
name	string	The full name of the module.
description	string	A description of the module's
		purpose (in other words, the
		calculations performed by the
		module).
domain	AstrophysicalDomain	The astrophysical domain into
		which the module has been
		sorted.
codeName	string	The name of the AMUSE class
		containing the module code.
codeLocation	string	The location of the AMUSE
		module code.
isParallel	boolean	Whether the module's
		calculations can be parallelized
		across multiple workers by MPI.
stoppingConditions	StoppingConditions	The condition(s) under which
		the module may stop executing
		prematurely.
parameters	List <parameter></parameter>	The module parameters. These
		module-specific values may be
		modified prior to running the
		experiment in order to fine-tune
		the module's behavior.

4.3.1.2 Module Operations

string get Namel I	void setName(string name)		
string getName() Input (none)	Input A new, full name for this		
Output The full name of the module.	Output (none)		
Description Returns the name of the module.	Description Updates this module's name to the given argument.		

string getDescription()		void setDescription(string description)		
Input	(none)	Input	A new description of this	
Output	A description of the		module's purpose and	
	module's purpose and		calculations performed.	
	the calculations it	Output	(none)	
	performs.	Description	Updates this module's	
Description	Returns this module's		descriptive text to the	
	descriptive text		given argument.	

AstrophysicalDomain getAstrophysicalDomain() void setAstrophysicalDomain(AstrophysicalDomain domain					
Input	(none)		Ing	out	An astrophysical domain
Output	The astrophysical				into which this module
-	domain into which the				will be sorted.
	module has been sorted.		Out	put	(none)
Description	Returns this module's		Descr		Updates this module's
	astrophysical domain.			•	astrophysical domain.
string	g getCodeName()	VC	oid setCode	Name	(string codeName)
Input	(none)		Input	The	name of an AMUSE
Output	The name of the		-	class	containing this
-	AMUSE class containing			mod	ule's code.
	this module's code.	C	utput	(nor	e)
Description	Returns the name of the		scription	Ùpd	ates this module's
_	module's associated		-	code	reference to the
	AMUSE class.			give	n argument.
string	getCodeLocation()	voi	d setCodeL	ocati	on(string codeLocation)
Input	(none)		Input		location of the
Output	The location of the			AMUSE code that	
	AMUSE code that			defir	es this module.
	specifies this module.	C	Output (none)		e)
Description	Returns the location of	De	escription Updates this module's		ates this module's
	the module's AMUSE		code location reference		
code.				to t	ne given argument.
boole	an getParallelism()	VC	void setParallelism(boolean isParallel)		(hoolean isParallel)
Input	(none)		Input		ther the module's
Output	Whether the module's		input		ulations can be
	calculations can be				llelized across
	parallelized across				iple workers by MPI.
	multiple workers by MPI.	-	utput	(nor	
Description	Returns a boolean		scription		or clears the
	indicating whether the	Je.	Cipaon		llelism flag for this
	module's calculations			mod	
	can be parallelized.				uic.
StoppingConditions getStoppingConditions() vo			void setS	toppii	gConditions(StoppingConditions conds)
Input	(none)		Input A bitfield indicating the		
Output	The conditions under		stopping conditions for		
	which this module may			this module.	
	stop executing	Output (none)			
	prematurely.	• • • • • • • • • • • • • • • • • • •		Updates this module's	
Description	Returns the stopping		stopping conditions to		• • •
	conditions specified for		those represented by the		· · · · · · · · · · · · · · · · · · ·
	the module.		given argument.		given argument

List / Paran	neter> getParameters()	void setParameters(List <parameter> parameters)</parameter>		
Input Output	(none) A list of the module's	Input Output	A list of module parameters. (none)	
Description	parameters. Returns the parameters of this module.	Description	Updates this module's parameter list to the given argument.	
		boolean remo	veParameter(Parameter p)	
void addP	arameter(Parameter p)	Input	A module parameter to remove from the module.	
Input	A module parameter to add to the module.	Output	Whether the given parameter was removed.	
Output Description	(none) Adds the given		Returns false if the parameter was not found in this module's	
	parameter to this module.	- Description	parameter list. Removes the given	
		Description	parameter from this module, if the parameter exists.	
		static Module fromXml(string element)		
	tring toXml()	Input	A string containing an XML representation of a	
Input Output	(none) A string containing an	Output	Module. A Module whose	
	XML representation of the Module.	Output	property values are specified by the given	
Description	Dumps the Module to an XML element.	Description	XML element. Recreates a Module from its XML	
			specification.	

4.3.2 Parameter Class

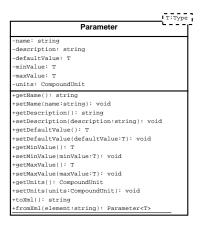


Figure 4.5: Parameter class diagram

Modules have parameters that may be modified by the user via the graphical interface. These parameters are typically specific to the module's domain or even to the individual module. The Parameter class is a generic class whose type parameter specifies the type of the parameter's value (e.g. integer or floating-point). A parameter may be a physical quantity, flag, or other value. (Satisfies Requirement 2.3.6)

4.3.2.1 Parameter Attributes

Name	Туре	Description
T	Туре	The data type of the parameter's value.
name	string	The brief, descriptive name of the parameter.
description	string	A description of the parameter's meaning and effects.
defaultValue	T	The parameter's default value.
minValue	Т	A lower bound on the range of valid parameter values.
maxValue	Т	An upper bound on the range of valid parameter values.
units	CompoundUnit	The physical unit(s) associated with the parameter's value.

4.3.2.2 Parameter Operations

string getName()		void setName(string name)		
		Input	A new name for this	
Input	(none)		parameter.	
Output	The brief, descriptive name of the parameter.	Output	(none)	
Description	Returns the name of the	Description	Updates this	
Description	parameter.		parameter's name to the given argument.	
		1	given argument.	

string getDescription()		void setDescription(string description)		
Input	(none)	Input	A new description for	
Output	A description of the		this parameter.	
	parameter's meaning	Output	(none)	
	and effects.	Description	Updates this parameter's	
Description	Returns this parameter's		descriptive text to the	
	descriptive text.		given argument.	
T or	etDefaultValue()	void setDefa	ultValue(T defaultValue)	
		Input A new default value for		
Input	(none) The parameter's default		this parameter.	
Output	value.	Output	(none)	
Description	Returns the default	Description	Updates this parameter's	
Description	value for this parameter.		default value to the	
	value for this parameter.		given argument.	
	mat Min Value ()	void set N	MinValue(T minValue)	
	getMinValue()	Input	A new lower bound on	
Input	(none)		this parameter's range	
Output	The parameter's		of possible values.	
	minimum valid value.	Output	(none)	
Description	Returns the minimal	Description	Updates this parameter's	
	allowed value for this		minimum value to the	
	parameter.		given argument.	
		void setMaxValue(T maxValue)		
	getMaxValue()	Input A new upper bound or		
Input	(none)	IIIput	this parameter's range	
Output	The parameter's		of possible values.	
	maximum valid value.	Output	(none)	
Description	Returns the maximal	Description	Updates this parameter's	
	allowed value for this	Bescription	maximum value to the	
	parameter.		given argument	
Compo	oundUnit getUnits()	., , ,	-	
Input	(none)		ts(CompoundUnit units)	
Output	An object representing	Input	A new compound	
Output	the physical unit(s)		physical unit to be	
	associated with the		associated with this	
parameter's value.			parameter	
Description	Returns an object	Output	(none)	
Description	containing the units	Description	Updates this	
	associated with this		parameter's units to the	
	parameter.		given argument.	
	F =	J		

		static Parameter <t> fromXml(string element)</t>		
		Input	A string containing an	
string toXml()			XML representation of a	
Input	(none)		Parameter.	
Output	A string containing an	Output	A Parameter whose	
	XML representation of		property values are	
	the Parameter.	specified by the given		
Description	Dumps the Parameter to		XML element.	
	an XML element.	Description Recreates a Parameter		
			from its XML	
	specification.		specification.	

4.3.3 Unit Class



Figure 4.6: Unit class diagram

With AMUSE, physical quantities may be expressed using, and converted between, a number of different standard units. The Unit class, in conjunction with the CompoundUnit class, allows GPUnit to present these units to the user for the purposes of description and selection.

4.3.3.1 Unit Attributes

Name	Туре	Description
type	UnitType	The base type of astrophysical unit being represented.
prefix	SIPrefix	The SI prefix that modifies the base unit's order of magnitude.
exponent	integer	The exponent to be applied to the unit. For example, a typical unit of volume (such as cubic meters) would have an exponent of 3.

		UnitType getType()		void setType(UnitType type)		
		Input	(none)	Input	A base astrophysical	
		Output	The base type of		unit to which this	
			astrophysical unit being		instance should be	
4.3.3.	2 Unit Operations		represented.		updated.	
		Description	Returns the base type of	Output	(none)	
			astrophysical unit	Description	Updates this instance's	
			represented by this		base unit type to the	
			instance.		given argument	
	SIPrefix getPr	efix()	void setPrefix(SIPre	efix prefix)		

SIPrefix getPrefix()		void setl	Prefix(SIPrefix prefix)
Input	(none)	Input	An SI prefix that will
Output	The SI prefix that modifies the base unit's		replace this instance's current SI prefix.
	order of magnitude.	Output	(none)
Description	Returns the SI prefix that augments the magnitude of this unit.	Description	Updates this instance's SI prefix to the given argument.
UnitType getExponent()			ponent(UnitType type)
Input	(none)	Input	A new exponent to be applied to this unit.
Output	The exponent applied to this unit.	Output	(none)
Description	Returns the exponent applied to this unit.	Description	Updates this instance's exponent to the given argument.

4.3.4 CompoundUnit Class

CompoundUnit	
-description: string -symbolicDescription: string -units: List <unit></unit>	
generation (): string (): string (): string (): void (): string (): void (): string ():	

Figure 4.7: CompoundUnit class diagram

When performing physical calculations, units of measure may combined in any number of ways. The CompoundUnit class provides the mechanism by which units may be presented to the user, regardless of whether they are simple or compound.

4.3.4.1 CompoundUnit Attributes

5.4.1 Compoundont Attributes			
Name	Туре	Description	
description	string	A non-abbreviated textual	
		description of the combined	
		physical unit	
symbolic Description	string	A shorthand textual description	
		of the combined physical unit,	
		using unit abbreviations.	
units	List <unit></unit>	The list of simple units whose	
		combination is represented by	
		this compound unit.	

	ŗ	strinę	g getDescription()		
	r	Input	(none)	void setDesc	ription(string d
	, i	Output	A non-abbreviated	Input	A new, full de
	ı	1	textual description of		for this comp
4.3.4.2	CompoundUnit Operations	1	the combined physical	Output	(none)
	ı	1	unit.	Description	Updates this
	ř	Description	Returns a textual		description to
	ı	1	description of this		argument.
	'	1	combined unit.		

		COII	ibilied uliit.
string getSymbolicDescription()		void setSymb	olicDescription(string symbolicDescription)
Input	(none)	Input	A new abbreviated
Output Description	A shorthand textual description of the combined physical unit, using unit abbreviations. Returns an abbreviated description of this combined unit.	Output Description	description for this compound unit. (none) Updates this instance's short description to the given argument.
List < Unit > getUnits()		void sattl	nits(List <unit> units)</unit>
Input (none)		Input	A list of simple units to
Output Description	The list of simple units whose combination is represented by this compound unit. Returns the list of units	Output Description	which this instance should be updated (none) Updates this instance's
Bescription	contained in this compound unit.	9	list of simple units to the given argument.

void	addUnit(Unit u)
Input A unit to be included in	
	this compound unit.
Output (none)	
Description Adds the given unit to	
	this compound unit's list
	of simple units.

	boolean removeUnit(Unit u)		
	Input A unit to remove from		
	this compound unit.		
╡	Output	Whether the given unit	
		was removed. Returns	
4		false if the unit was not	
4		found in this instance's	
	unit list.		
ſ	Description Removes the given		
4	simple unit from this		
	compound unit, if the		
		simple unit exists.	

4.3.5 UnitType Enumeration



Figure 4.8: UnitType type diagram

UnitType enumerates the myriad of base physical units supported by AMUSE. The list of members shown may not be exhaustive.

4.3.6 SIPrefix Enumeration

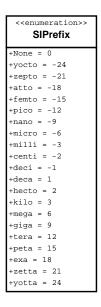


Figure 4.9: SIPrefix type diagram

When dealing with physical quantities, standard prefixes may be prepended to units to denote a given quantity's order of magnitude. SIPrefix enumerates the possible unit prefixes.

4.3.7 Astrophysical Domain Enumeration

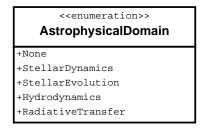


Figure 4.10: Astrophysical Domain type diagram

The modules included with AMUSE have categorized according to their domain. A module's domain indicates the quantities it deals with as well as common operations that may be called on the module. The AstrophysicalDomain type enumerates the several domains that have been specified by AMUSE.

4.3.8 StoppingConditions Enumeration

<<enumeration>> StoppingConditions +None = 0 +Collision = 1 +Pair = 2 +Escaper = 4 +Timeout = 8 +NumberOfSteps = 16 +OutOfBox = 32

Figure 4.11: StoppingConditions type diagram

StoppingConditions is a set of bit flags enumerating the conditions under which a module may return from execution before completing its assigned calculations.

4.4 Diagnostics

Diagnostics have access to the state of the experiment at the end of each time step. Default diagnostics will be provided, e.g. printing the state to a file at a specified time step or creating a stellar mass histogram. Users can create custom diagnostic plug-ins. (Satisfies requirement 2.6)

4.4.1 Object Model

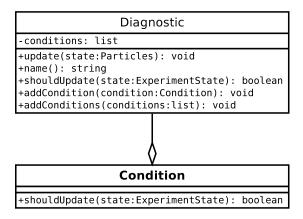


Figure 4.12: Diagnostics Object Model

4.4.2 Diagnostic Class

The Diagnostic class is an abstract class that is the base of both built-in and custom diagnostics tools. All custom diagnostic scripts must inherit from this class. Subclasses must implement the update and name operations. The Diagnostic class also contains a list of conditions to check if the diagnostic needs to be updated.

4.4.3 Experiment Manager Class

The Experiment Manager class has the responsibility to manage as well as update the active diagnostics.

4.4.4 Condition Class

The Condition class represents the conditions that need to be satisfied for a diagnostic to be updated.

4.5 Logging

Logs are helpful when the experiment must be restarted along with its output data if the experiment has an error or needs to be stopped for any other reason. Logging could be enabled or disabled by the user. The output destination for the logs could be specified. The specified destination for the output can be one among the following: the console, a file, or a window in the GUI. (Satisfies requirement 2.7)

4.5.1 Object Model

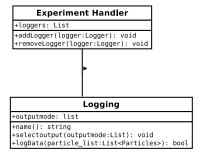


Figure 4.13: Logging Object Model

4.5.2 Logging Class

The Logging class takes care of selecting the required output option as the console, file or the GUI window.

5 Command Line Tool

5.1 Overview

The command line tool (CLT) is used for the running of an experiment file. The CLT begins with parsing the experiment file. After parsing the experiment file the CLT takes the initialization parameters and loads them using the AMUSE framework. The CLT then takes the modules specified, searches through loaded AMUSE modules and initializes the modules. The CLT links the modules together to allow interaction and updating of the current state of the system using the AMUSE channels. The CLT then loads the Logging and Data Analysis scripts specified by the experiment file, linking it to the the particle array. The CLT then runs through the time specified in the experiment file, evolving all of the modules loaded at each time step. It will run the data analysis scripts as well as the logging on the intervals specified. After the model is done evolving it will output using whatever data analysis script listed, in the file format specified.

5.2 Using the CLT

The command line tool will primarily be used by the GUI to send out jobs and run them to make the user experience much more enjoyable and at ease. The command line tool though can be used with a basic experiment file with some on the fly modifications by using some flags. (Satisfies requirement 2.4.1)

5.2.1 CLT Flags

Flag	<value being="" passed=""></value>	Description	
-help	None	Displays a useful help prompt with the list of CLT flags.	
-f	Experiment File Location	Loads the experiment file prompted by the filename.	
-n	Number of Particles	Changes the number of particles being passed in the experiment file.	
-t	End Time	Changes the max time allowed in the simulation.	
-dt	Timestep	Changes the timestep in which dt moves forward.	
-r	Radius	Changes the radius scaling factor.	

5.3 Running The Experiment

5.3.1 Simulation Overview

A Simulation is the goal of both GPUnit and AMUSE, which makes it important to understand and break it into key parts. The Simulation can be looked at as three sections: Simulation Initialization, Running Simulation, Post Simulation. This section will go into more detail about all three of these parts and what happens in each.

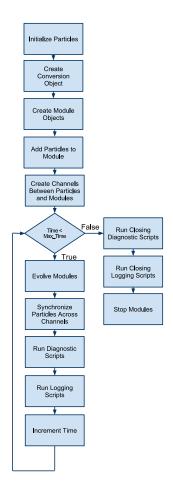


Figure 5.1: Flow Chart of Typical AMUSE Simulation

- **5.3.1.1 Simulation Initialization** Simulation Initialization is used for preparation of the particles and modules to be able to model the system. The following will break down the initialization into the main steps.
- **5.3.1.1.1 Instantiate Particles** In the initialization phase of the experiment it is important to select proper initial conditions. The main initial conditions to set is the mass distribution and and starting locations of the particles. There are built in AMUSE classes that are used to set these. The CLT while reading in the experiment file will find the initial condition files by name. (Satisfies Requirements 2.3.4)
- **5.3.1.1.2 Create Conversion Object** Most astronomical simulations use a scaling factor so you can do the numerical integration quicker. A conversion object is

a class in AMUSE that you instantiate by passing in the total mass and the average radius of the system. You will then pass this conversion object into any modules you will be using in the future so the module knows how to translate between this smaller number format to an actual real data value.

- **5.3.1.1.3 Module Creation** The CLT needs to instantiate the AMUSE class for the specific module it is working on from the location specified in the module class. It needs to instantiate the module being passed in the conversion object so the module knows what units it is working in and how to convert its units. The module then sets its list of particles to the master list of particles. After it does that it needs to run it's initial calculations needed for evolving the module.
- **5.3.1.1.4** Instantiate Channels Channels are used to be able to communicate data to and from the modules that may be on a different system. On every time step you need to synchronize the master list of particles to every modules separate list of nodes. Afterwards you need to re-sync the modules nodes to the master node. This allows the modules to have the same data to move forward in the simulation. (Satisfies Requirement 2.5.1, 2.5.2, 2.5.2.1)
- **5.3.1.2** Running Simulation Running the system is the area inside of the while loop. This is where the modules are run, some logging is done, some diagnostics and increment the time scale. (Satisfies Requirement 2.4.2)
- **5.3.1.2.1 Evolve Modules** The evolution of the Module is core of running a simulation. The evolution of the module is done by running the AMUSE module's evolve model function with passing in the current time.
- **5.3.1.2.2 Synchronize Particles** Synchronize particles is required due to the fact every module has a local list of particles to allow parallelization. These particles are updated, yet only one set of dynamics or stellar evolution will be run at a time which prevents any overlapping of data modification. To synchronize the particles you run all the channels created to synchronize all the data to the master list of particles. After the master list is up to date, you then synchronize using all the channels to the modules. This leaves all the modules' list of particles with the latest version of particle data.
- **5.3.1.2.3** Run Diagnostics The function should loop through all the diagnostic scripts and if the diagnostics should use the shouldUpdate function with the current state of the experiment to check if it should run. If the diagnostic should run, it then runs the update method passing in the master list of particles.(Figure 4.12)

- **5.3.1.2.4** Run Logging The function will loop through all the logging scripts and run any real time logging scripts that need to be run. The real time logging scripts are denoted by name and run their logData method passing in the list of particles.(Figure 4.13)
- **5.3.1.2.5** Increment Time The time should increment using the specified timestep (Figure 4.1). The stopping of the experiment is signaled when the stopping conditions are met. (Satisfies Requirement 2.4.3.1)

5.3.1.3 Post Simulation

- **5.3.1.3.1** Run Closing Diagnostics Scripts The function should loop through all the diagnostic scripts and if the diagnostics should use the shouldUpdate function with the current state of the experiment to check if it should run. If the diagnostic should run, it then runs the update method passing in the master list of particles.(Figure 4.12)
- **5.3.1.3.2** Run Closing Logging Scripts The function will loop through all the logging scripts and run any post simulation logging scripts that need to be run. The post simulation logging scripts are denoted by name and run their logData method passing in the list of particles. (Figure 4.13)
- **5.3.1.3.3 Stop Modules** The modules should be cleaned up after being run. This involves if running in parallel sending a kill command via MPI. We will run the modules' (AMUSE class) stop() command.

6 Networking

6.1 Overview

The networking layer is responsible for communication between the interface and the cluster status daemons running on the cluster nodes. The user interface and console can send messages through the network which will be distributed via IP multicast to any cluster nodes listening to a selected multicast group. Cluster nodes will be able to send replies to the sender containing information such as health stats and the number of experiments running on that node. The UI and command line tools will use IPC (pipes etc...) to communicate with local instances of the control program to send network packets to the cluster nodes.

6.2 Network Software Components

6.2.1 Control Instance

A control instance is a program that will run in the background on any machine wishing to control experiments on a cluster. The core scripts (command line tools)

and UI will both communicate with this instance to perform any network access.

6.2.2 Node Instance

Node instances are processes that run on each computing node in the cluster. The node instance tracks health statistics and running experiments and can send these pieces of information as direct (unicast) replies to queries received through the multicast group.

6.3 Object Model

6.3.1 Overview

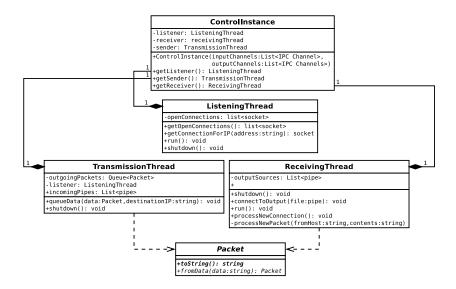


Figure 6.1: Network Object Model

6.3.2 Control Instance

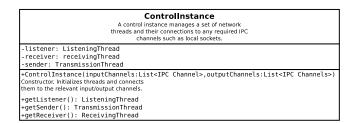


Figure 6.2: Control Instance Class Diagram

6.3.3 Node Instance

NodeInstance

A node instance runs once on each node in the cluster that needs to be managed. Each node instance listens for multicast packets and replies to requests for information.

-nodeName: string

The name of the node that will be returned if requested in a status query.

+NodeInstance(multicastGroupIP:string, nodeName:string)
Constructor called when the node instance is
started. It connects to the desired multicast
group and listens for requests.

Figure 6.3: Node Instance Class Diagram

6.3.4 TransmissionThread

The transmission thread (Figure 6.4) will process outgoing packets queued for transmission by external sources such as the UI.

TransmissionThread

The transmission thread listens to a set of IPC channels and gathers strings that need to be sent to other machines. These strings are then sent out over the network, establishing a connection if needed.

-outgoingPackets: Queue<Packet>

Thread-local queue of Packets that other threads/programs have queued to send.

-listener: ListeningThread

The TransmissionThread needs access to the listener in order to access established connections.

+incomingPipes: List<pipe>

Programs that wish to send data can place the packet strings into one of these pipes. The transmission thread will collect the strings and

send them to the destination.

+queueData(data:Packet,destinationIP:string): void
+shutdown(): void

Figure 6.4: Transmission Thread Class Diagram

6.3.5 ReceivingThread

The receiving thread (Figure 6.5) will read incoming packets from established connections with node instances.

ReceivingThread The receiving thread collects sockets from the listener and performs select() calls on them to gather incoming packets. These packets are distributed to any other programs on the system that need them, via IPC channels. outputSources: List<pipe> Programs that need to be notified of incoming traffic can connect to a pre-defined pipe to receive data from the network. These pipes are stored in the receiver thread so it can send copies of each packet to the programs on the other side of the pipe. +shutdown(): void Cleanly shutdown the thread, closing any established connections. +connectToOutput(file:pipe): void Adds the specified file descriptor to a list of file descriptors that need data from the eceiving thread. run(): void +processNewConnection(): void When a new connection is established in the listener, it uses this method to inform the receiver that it needs to add this connection to the list of potential remote senders. -processNewPacket(fromHost:string,contents:string) Handles received data from a single host, called whenever the thread receives new data from a onnection.

Figure 6.5: Receiving Thread Class Diagram

6.3.6 ListeningThread

The listening thread (Figure 6.6) will listen for and accept new incoming connections from node instances.

ListeningThread The listener thread will run accept() in a loop and pass off new sockets to the receiver thread which will select/read the sockets to collect data. -openConnections: list<socket> +getOpenConnections(): list<socket> Returns a list of all connections accepted by this listener. +getConnectionForIP(address:string): socket Given an IP address, this finds the corresponding socket for that connection and returns it. +run(): void +shutdown(): void Cleanly shuts down the thread, closing any open connections.

Figure 6.6: Listening Thread Class Diagram

6.3.7 Packet Objects

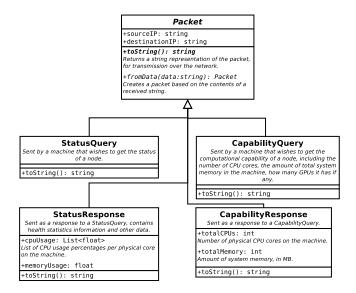


Figure 6.7: Packet Classes

7 Data

7.1 Experiment Specification

The following is a list of XML specifications for experiments. Experiments are saved and loaded via this format. Note that not all specified attributes will always be present because not all attributes are relevant to every experiment. See Figure 7.1 for an example XML experiment file. (Satisfies requirement 2.3.3, 2.3.5)

Figure 7.1: Example XML Experiment File

7.1.1 Experiment

Experiment tags are the first and last tags in an experiment specification because they encapsulate all experiment attributes.

Attribute	Description
name	The name of the experiment

7.1.2 Time

Time tags specify the time parameters of the experiment.

Attribute	Description
units	The time units for the experiment to use, defined by AMUSE
start	The start time of the experiment
step	The amount of time between simulation snapshots
end	The time to end the experiment

7.1.3 Module

Module tags define the modules used in the experiment. Each module has child param tags to define initial conditions. These initial conditions are defined by AMUSE.

٧,	O	
	Attribute	Description
	name	The name of the module to use

714 Param

Param tags define the parameters for their parent model. Each defines a model's parameter value for use in the experiment. All parameters, default values, units, and descriptions are defined by AMUSE.

Attribute	Description
name	The name of the parameter to initialize
value	The value to give the parameter

7.1.5 Particle

Particle tags define the particles used in the experiment. All references to units are those defined by AMUSE.

Attribute	Description
mass	The mass of the particle with units
radius	The radius of the particle with units
position	The position of the particle in $[X,Y,Z]$ format with units
velocity	The velocity of the particle in $[X,Y,Z]$ format with units
luminosity	The luminosity of the particle with units
temperature	The temperature of the particle with units
age	The age of the particle with units
stellarType	The stellar type of the particle, defined by AMUSE

7.1.6 Diagnostic

Diagnostic tags define the diagnostic scripts used in the experiment.

	Attribute Description		
name T		The name of the diagnostic for reference purposes	
	file	The filename of the diagnostic script	

7.1.7 Logger

Logger tags define the logging scripts used in the experiment.

Attribute	Description	
name The name of the logger for reference purpose file The filename of the logging script		

7.1.8 Stopping Condition

Stopping Condition tags define the stopping conditions used in the experiment. All stopping conditions are defined by AMUSE.(Satisfies Requirement 2.4.3, 2.4.3.2)

	,
Attribute	Description
type	The type of stopping condition to use

7.2 Network Packets

The following is a list of packet data content specifications. Data is described in terms of types to ease implementation, however the information is sent over the network as a string to avoid any machine-specific byte ordering issues. Fields in the packet are separated by a "|" character. If this character is to appear as text inside a packet for any reason, it must be escaped as "\|"

7.2.1 Packet Header

The packet header precedes data in all packets.

PACKET_TYPE	LENGTH	SOURCE_IP	DEST_IP
int	long	string	string

7.2.2 Status Query Packet

The status request may contain flags requesting additional data from the node beyond the elements specified here. If the recipient understands the flags, they will fill the ADDITIONAL_DATA field with the appropriate response.

	_		
HEADER	ADDITIONAL_	_REQUEST_	_FLAGS
-		string	

7.2.3 Status Response Packet

HEADER	CPU_USAGE	MEMORY_USAGE	SIMS_RUNNING	ADDITIONAL_DATA
-	float	float	string	string

7.2.4 Capability Query Packet

The additional data protocol is the same here as in the status request above.

HEADER	ADDITIONAL_REQUEST_F	LAGS
-	string	

7.2.5 Capability Response Packet

HEADER	NUM_CPUS	MAX_MEMORY	NUM_GPUS	ADDITIONAL_DATA
-	int	long	int	string

8 Appendix

8.1 Requirements Traceability Table

Requirement	Section in SDD
2.2.1	4.3.1
2.2.2	4.3.1
2.2.3	4.3.1
2.2.4	4.3.1
2.2.5	4.3.1
2.3.1	4.2
2.3.2	4.2
2.3.3	4.1
2.3.4	5.3.1.1.1
2.3.5	7.1
2.3.6	4.3.2
2.4.1	5.2
2.4.2	5.3.1.2
2.4.3	5.3.1.2.5
2.4.4	5.3.1.2.5
2.5.1	5.3.1.1.4
2.5.2	5.3.1.1.4
2.6.1	4.4
2.6.2	4.4
2.6.3	4.4
2.6.4	4.4
2.6.5	4.4
2.6.6	4.4
2.7.1	4.5
2.7.2	4.5
2.7.3	4.5
2.8.1	3.3
2.8.2	3.3

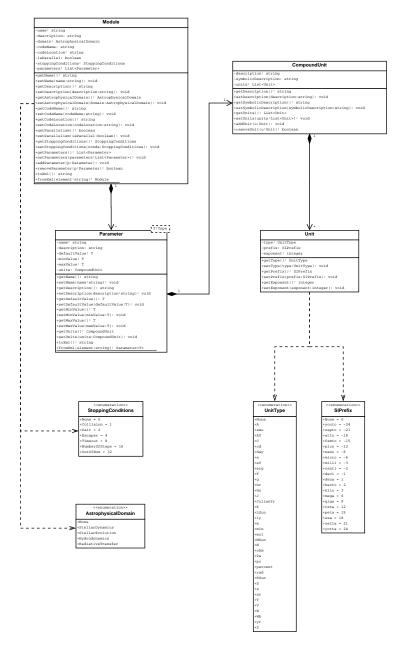


Figure 4.3: Relationships between Module and supporting classes