# Biomolecular Sequence Analysis Specification, V1.0

This OMG document replaces the draft adopted specification and the submission documents. It is an OMG Final Adopted Specification, which has been approved by the OMG board and technical plenaries, and is currently in the finalization phase. Comments on the content of this document are welcomed, and should be directed to *issues@omg.org* by December 4, 2000.

You may view the pending issues for this specification from the OMG revision issues web page *http://www.omg.org/issues/*; however, at the time of this writing there were no pending issues.

The FTF Recommendation and Report for this specification will be published on January 8, 2001. If you are reading this after that date, please download the available specification from the OMG formal specifications web page.

OMG Adopted Specification November, 2000

# Biomolecular Sequence Analysis Specification

**Final Adopted Specification** November 2000 Copyright 1999, Concept Five Technologies, Inc. Copyright 1999, EMBL-EBI (European Bioinformatics Institute) Copyright 1999, Genome Informatics Corporation Copyright 1999, Millennium Pharmaceuticals, Inc. Copyright 1999, Neomorphic Software, Inc. Copyright 1999, NetGenics, Inc.

The companies listed above have granted to the Object Management Group, Inc. (OMG) a nonexclusive, royalty-free, paid up, worldwide license to copy and distribute this document and to modify this document and distribute copies of the modified version. Each of the copyright holders listed above has agreed that no person shall be deemed to have infringed the copyright in the included material of any such copyright holder by reason of having used the specification set forth herein or having conformed any computer software to the specification.

#### PATENT

The attention of adopters is directed to the possibility that compliance with or adoption of OMG specifications may require use of an invention covered by patent rights. OMG shall not be responsible for identifying patents for which a license may be required by any OMG specification, or for conducting legal inquiries into the legal validity or scope of those patents that are brought to its attention. OMG specifications are prospective and advisory only. Prospective users are responsible for protecting themselves against liability for infringement of patents.

#### NOTICE

The information contained in this document is subject to change without notice. The material in this document details an Object Management Group specification in accordance with the license and notices set forth on this page. This document does not represent a commitment to implement any portion of this specification in any company's products.

WHILE THE INFORMATION IN THIS PUBLICATION IS BELIEVED TO BE ACCURATE, THE OBJECT MANAGEMENT GROUP AND THE COMPANIES LISTED ABOVE MAKE NO WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, WITH REGARD TO THIS MATERIAL INCLUDING, BUT NOT LIMITED TO ANY WARRANTY OF TITLE OR OWNERSHIP, IMPLIED WARRANTY OF MERCHANTABILITY OR WARRANTY OF FITNESS FOR PARTICULAR PURPOSE OR USE. In no event shall The Object Management Group or any of the companies listed above be liable for errors contained herein or for indirect, incidental, special, consequential, reliance or cover damages, including loss of profits, revenue, data or use, incurred by any user or any third party. The copyright holders listed above acknowledge that the Object Management Group (acting itself or through its designees) is and shall at all times be the sole entity that may authorize developers, suppliers and sellers of computer software to use certification marks, trademarks or other special designations to indicate compliance with these materials. This document contains information which is protected by copyright. All Rights Reserved. No part of this work covered by copyright herein may be reproduced or used in any form or by any means--graphic, electronic, or mechanical, including photocopying, recording, taping, or information storage and retrieval systems--without permission of the copyright owner.

RESTRICTED RIGHTS LEGEND. Use, duplication, or disclosure by government is subject to restrictions as set forth in subdivision (c) (1) (ii) of the Right in Technical Data and Computer Software Clause at DFARS 252.227.7013 OMG<sup>®</sup> and Object Management are registered trademarks of the Object Management Group, Inc. Object Request Broker, OMG IDL, ORB, CORBA, CORBAfacilities, CORBAservices, COSS, and IIOP are trademarks of the Object Management Group, Inc. X/Open is a trademark of X/Open Company Ltd.

#### ISSUE REPORTING

All OMG specifications are subject to continuous review and improvement. As part of this process we encourage readers to report any ambiguities, inconsistencies, or inaccuracies they may find by completing the issue reporting form at *http://www.omg.org/library/issuerpt.htm*.

# Contents

	Prefac	e		1
	Abou	t the Object	t Management Group	1
		What is CO	DRBA?	1
	Asso	ciated OMC	Documents	2
	Ackn	owledgmen	ts	2
1.	Overv	iew		1-1
	1.1	Module D	DsLSRBioObjects	1-1
	1.2	Module D	OsLSRAnalysis	1-2
	1.3	Domain N	Aodel	1-2
	1.4	General R	Remarks	1-2
		1.4.1	Objects-by-value	1-2
		1.4.2	Returning Multiple Results	1-3
		1.4.3	Identifier	1-3
		1.4.4	Composite Pattern.	1-3
		1.4.5	BioObject Immutability	1-4
		1.4.6	Rationale for Metadata Approach	1-4
2.	BSA N	<b>Iodules</b> ar	nd Interfaces	2-1
	2.1	Module D	DsLSRBioObjects	2-1
		2.1.1	General	2-2
		2.1.2	StrandType	2-3
		2.1.3	Basis	2-4
		2.1.4	Interval	2-5
		2.1.5	SeqRegion	2-6
		2.1.6	Annotation	2-10

		2.1.7	SeqAnnotation	2-14
		2.1.8	Identifier	2-18
		2.1.9	BioSequence	2-22
		2.1.10	Sub-types of BioSequence	2-29
		2.1.11	CodeRule	2-34
		2.1.12	GeneticCode	2-37
		2.1.13	AlignmentElement	2-38
		2.1.14	AlignmentElementIterator	2-41
		2.1.15	Alignment	2-42
		2.1.16	Alignment Examples	2-51
		2.1.17	Assembly	2-53
		2.1.18	SearchHit	2-54
		2.1.19	SimilaritySearchHit	2-57
		2.1.20	BioSequenceIdentifierResolver	2-59
		2.1.21	SearchResult	2-60
		2.1.22	AnnotationFactory (Optional)	2-64
		2.1.23	BioSequence factories (Optional)	2-66
		2.1.24	BioSequence iterators (Optional)	2-70
		2.1.25	GeneticCodeFactory (Optional)	2-74
		2.1.26	CharacterAlignmentEncoder (Optional)	2-76
		2.1.27	SingleCharacterAlignmentEncoder (Optional).	2-81
		2.1.28	AlignmentEncoder factories (Optional)	2-83
	2.2	Module D	sLSRAnalysis	2-85
		2.2.1	General	2-86
		2.2.2	AnalysisType	2-87
		2.2.3	InputPropertySpec	2-89
		2.2.4	OutputPropertySpec	2-91
		2.2.5	AnalysisState	2-92
		2.2.6	AnalysisEvent	2-93
		2.2.7	Sub-types of AnalysisEvent	2-94
		2.2.8	AnalysisService	
		2.2.9	JobControl	
		2.2.10	AnalysisInstance	
		2.2.11	Sequence Diagrams	2-108
3.	Domai	n Model .		3-1
	3.1	Metadata.		3-1
		3.1.1	Role of XML	3-1
		3.1.2	Role of DTD	3-2
		3.1.3	Domain Metadata	3-3
	3.2	Classificat	ion of Analyses	3-6

# **Contents**

	3.2.1	Searching	3-6
	3.2.2	Alignment	3-6
	3.2.3	Utilities	3-6
Appendix	x A - Ref	erences	A-1
Appendiz	x B - Ger	netic Codes	B-1
Appendiz	x C - Cor	nplete IDL	C-1
Appendix	x D - Doi	main Model DTD and XML	D-1
Appendiz	x E - Futi	ure Direction of Metamodel	E-1
Glossary		Gloss	sary-1

# Preface

# About the Object Management Group

The Object Management Group, Inc. (OMG) is an international organization supported by over 800 members, including information system vendors, software developers and users. Founded in 1989, the OMG promotes the theory and practice of object-oriented technology in software development. The organization's charter includes the establishment of industry guidelines and object management specifications to provide a common framework for application development. Primary goals are the reusability, portability, and interoperability of object-based software in distributed, heterogeneous environments. Conformance to these specifications will make it possible to develop a heterogeneous applications environment across all major hardware platforms and operating systems.

OMG's objectives are to foster the growth of object technology and influence its direction by establishing the Object Management Architecture (OMA). The OMA provides the conceptual infrastructure upon which all OMG specifications are based.

# What is CORBA?

The Common Object Request Broker Architecture (CORBA), is the Object Management Group's answer to the need for interoperability among the rapidly proliferating number of hardware and software products available today. Simply stated, CORBA allows applications to communicate with one another no matter where they are located or who has designed them. CORBA 1.1 was introduced in 1991 by Object Management Group (OMG) and defined the Interface Definition Language (IDL) and the Application Programming Interfaces (API) that enable client/server object interaction within a specific implementation of an Object Request Broker (ORB). CORBA 2.0, adopted in December of 1994, defines true interoperability by specifying how ORBs from different vendors can interoperate.

# Associated OMG Documents

The CORBA documentation is organized as follows:

- *Object Management Architecture Guide* defines the OMG's technical objectives and terminology and describes the conceptual models upon which OMG standards are based. It defines the umbrella architecture for the OMG standards. It also provides information about the policies and procedures of OMG, such as how standards are proposed, evaluated, and accepted.
- CORBA: Common Object Request Broker Architecture and Specification contains the architecture and specifications for the Object Request Broker.
- *CORBAservices: Common Object Services Specification* contains specifications for OMG's Object Services.

The OMG collects information for each specification by issuing Requests for Information, Requests for Proposals, and Requests for Comment and, with its membership, evaluating the responses. Specifications are adopted as standards only when representatives of the OMG membership accept them as such by vote. (The policies and procedures of the OMG are described in detail in the *Object Management Architecture Guide.*)

OMG formal documents are available from our web site in PostScript and PDF format. To obtain print-on-demand books in the documentation set or other OMG publications, contact the Object Management Group, Inc. at:

OMG Headquarters
250 First Avenue, Suite 201
Needham, MA 02494
USA
Tel: +1-781-444-0404
Fax: +1-781-444-0320
pubs@omg.org
http://www.omg.org

# Acknowledgments

The following companies submitted and/or supported parts of this specification:

- Concept Five Technologies, Inc.
- EMBL-EBI (European Bioinformatics Institute)
- Genome Informatics Corporation
- Millennium Pharmaceuticals, Inc.
- Neomorphic Software, Inc.
- NetGenics, Inc.
- Oxford Molecular Group
- Sanger Centre

# Overview

### Contents

This chapter contains the following sections.

Section Title	Page
"Module DsLSRBioObjects"	1-1
"Module DsLSRAnalysis"	1-2
"Domain Model"	1-2
"General Remarks"	1-2

The domain of biomolecular sequence analysis comprises the sub-domains of biological objects and analysis mechanisms. The modules that address these areas are described in the following sections.

# 1.1 Module DsLSRBioObjects

Biological objects that are central to this specification include **BioSequence**, which is specialized into **NucleotideSequence** and **AminoAcidSequence**. An **Annotation** object is provided, which is specialized into **SeqAnnotation** for usage with **BioSe-quences**. **SeqAnnotations** can apply to specific parts of a sequence, and the mechanism to refer to these regions is provided by **SeqRegion** and **Interval**. **CompositeSeqRegion** provides the ability to nest **SeqRegions**. **GeneticCode**, associated with an organism, is an auxiliary object needed when translating sequences. The interface **Alignment** and ancillary types are used for representing comparisons between sequences or sequence families. It is also used in describing **SimilaritySearch-Hits** (i.e., matches found in sequence database, and **Assemblies**). **SearchHit** and **SearchResult** are used primarily for representing the results of similarity searches (e.g., BLAST).

The **Annotation** factory, the **BioSequence** iterators and factories, **SeqAnnotation** iterator, **GeneticCode** factory, and **AlignmentEncoders** and factories are optional interfaces.

The **Annotation** factory, the **BioSequence** iterators and factories, **GeneticCode** factory, and **AlignmentEncoders** and factories are optional interfaces.

# 1.2 Module DsLSRAnalysis

The **DsLSRAnalysis** module defines the components for supporting sequence analysis through a generic analysis design. The module provides the means to interrogate analyses inputs, output, and functionality. An analysis can be executed asynchronously as well as synchronously based on the client invocation. Executing analyses can be monitored by subscribing to an event channel or polling for state.

# 1.3 Domain Model

The domain model is expressed in XML. The domain model includes a simple classification of analyses. This is in response to the mandatory requirement of the RFP, and serves to organize the analyses into groups in a way that matches closely with how researchers and bioinformaticists think about and utilize such analyses.

This classification of analyses consists of three broad categories.

- Searching including similarity searching (e.g., BLAST)
- Alignment including contig assembly
- Utilities including molecular weight and GC content

# 1.4 General Remarks

This document contains a proposal for a standard that addresses the representation of a number of biological objects, as well as mechanisms for analyzing them. A few design principles and patterns that we have used are outlined first.

# 1.4.1 Objects-by-value

This document makes extensive use of objects-by-value (OBV, OMG Document orbos/98-01-18). This is a new OMG standard for the so-called **valuetype**, which is an entity that is halfway between an IDL **interface** and an IDL **struct**. They are not yet widely supported by all ORBs, but we think they are a very useful construct, as they promise to provide:

- choice: the client can choose to make the object 'local' or leave it remote,
- better scalability: only a single round trip transfers the whole state of the object,
- extendibility through inheritance,
- null value semantics.

We have used OBV **valuetypes** essentially as if they were extendible structs, using the following constraints:

• no methods

- all members / attributes are public
- inheritance only of valuetypes (no "supports SomeInterface").

**Note** – Factory methods were not used in the valuetypes. See the appropriate language mapping specifications for details on using ValueFactories.

#### 1.4.2 Returning Multiple Results

If a method has to return a multi-valued result to the caller, there is a design choice of returning these elements directly as a list, or through an iterator, or using a combination of both. We have adopted the latter, hybrid approach to allow the client to choose between the convenience of directly returned lists and the scalability of iterators. The methods having a multi-valued result use have:

- a list return type,
- a parameter in unsigned long how\_many,
- a parameter out AnIterator the\_rest.

The client specifies that it wishes to receive a list of no more than **how\_many** elements as the direct result. The remaining elements, if any, can be retrieved through the iterator returned in the **out** parameter. The iterators allow the retrieval of one element at a time, or several at once. This pattern was in fact taken directly from the **CosPropertyService**, and provides maximum flexibility to client programs.

A multi-valued result, either returned directly or through an iterator, is guaranteed not to contain duplicates. If a multi-valued result type is ordered and iterators are involved, the ordering is the same as that achieved by not having used any iterators.

### 1.4.3 Identifier

Many entities in molecular biology require ID strings, usually to uniquely identify it in a certain context. The current document also uses strings for ID attributes, but constrains their syntax and semantics to improve interoperability. To make the intended use of these strings clearer,

#### typedef string Identifier;

is provided and used in this specification.

# 1.4.4 Composite Pattern

The **CompositeSeqRegion** valuetype implements the Composite design pattern [Gamma et al., 1995]. This pattern composes entities into tree structures to represent hier-

1

archies. The Composite pattern treats individual objects and composites uniformly.

A biological example using the Composite pattern is a gene being composed of coding regions from a set of exons.

# 1.4.5 BioObject Immutability

All BioObjects in this specification, with the single exception of **BioSequence**, are immutable. Modifying other BioObjects is considered out of scope for sequence analysis, as defined by the RFP. Since it is clear that the results of many sequence analyses produce information that is frequently attached to sequences as annotations, we do provide the **add\_annotation()** method in **BioSequence**.

Implementors are free to choose to support mutable BioObjects, taking responsibility for the associated life cycle issues.

# 1.4.6 Rationale for Metadata Approach

A number of the initial submissions to the RFP for sequence analysis explored the use of metadata to describe the various types of sequence analyses that might be available to a client. In response to the RFP requirement for the specification of a domain model for sequence analysis, the metadata approaches varied from string descriptors, structs, and arrays of structs to well defined IDL interfaces.

In the process of preparing this RFP response the submitters considered a number of viable approaches to metadata for sequence analyses. There was a strong desire to leverage existing solutions if possible. A predecessor to this specification described the metadata model using valuetype based extensible structs. This approach is carried into the current specification. In recognition of the increasing use of XML to provide data descriptions for application metadata, the specification was enhanced to also support retrieval of XML based metadata. An XML DTD defining the metadata model has been introduced as well. Additionally the mechanism used to fetch metadata descriptions for analyses has been enhanced to support the introduction of new XML based metadata by supplying a tag that identifies the type of metadata described. It is expected that this tag-based retrieval approach could be used to provide access to OCL, XMI, or other formatted metadata in the future. In particular the submitters would have liked to leverage XMI for metadata description but, in the absence of clear examples of its use, chose to adopt a model based on our previous joint submission and to provide for extension in the future.

# BSA Modules and Interfaces

### Contents

This chapter contains the following sections.

Section Title	Page
"Module DsLSRBioObjects"	2-1
"Module DsLSRAnalysis"	2-85

# 2.1 Module DsLSRBioObjects

The analysis of biomolecular sequence information takes place within the broader domain of computational biology. This domain presents a very heterogeneous, rapidly evolving environment that has proven difficult to standardize. To offer a design that is both complete and practical for the field of sequence analysis, this specification includes an IDL specification for **Annotations** and so-called **SeqAnnotations**, which can be likened to Features in the DDBJ/EMBL/GenBank flat file format. These two data components serve to incorporate and organize additional information relevant to the sequence data. Examples include organism source information, biological descriptors, cross-references, molecular characterizations, known sites and variations within the sequence, bibliographic references, and relations to known diseases. **Annotations** and **SeqAnnotations** can also be attached to a sequence to carry new information that is computationally inferred, or experimentally determined. We believe that it is necessary to offer users an easy, extensible interface to organize and link this resulting information to biomolecular sequences either as whole-sequence **Annotations** or region-specific **SeqAnnotations** (Features).

Some of the entities described below use generic types such as **Any** or name-value pairs. It is deemed outside the scope of this document to standardize the types of values that can be contained in these generic types.

Existing standards that can be represented with the current proposal and to some extent have shaped it are: the NCBI datamodels; the DDBJ/EMBL/GenBank Feature Table Document; various sequence file formats (Fasta, EMBL/GenBank, GCG), and various sequence analysis tools (BLAST, FastA, Smith-Waterman, ClustalW, Wise2, Grail, the GCG suite).

The alignment portion of the response is aimed to effectively model all types of **BioSequence** and **BioSequence** related alignment problems in biomolecular sequence analysis. This ranges from the relatively simple cases of a pairwise alignment of two DNA sequences, to the complex case of a profile-HMM compared to genomic DNA.

# 2.1.1 General

//File: DsLSRBioObjects.idl

#ifndef \_DS\_LSR\_BIOOBJECTS\_IDL\_ #define \_DS\_LSR\_BIOOBJECTS\_IDL\_

#pragma prefix "omg.org"

#include <CosLifeCycle.idl>
#include <CosPropertyService.idl>

module DsLSRBioObjects

{ // ... };

#endif // \_DS\_LSR\_BIOOBJECTS\_IDL\_

#### #pragma prefix "omg.org"

To prevent name space pollution and name clashing of IDL types, this module (and all modules defined in this specification) uses the pragma prefix that is the OMG's DNS name.

#include <CosLifeCycle.idl>

NucleotideSequence, AminoAcidSequence, Annotation, GeneticCode, Alignment, and SearchResult all inherit from LifeCycleObject.

#include <CosPropertyService.idl>

Properties are used in Annotation, SearchHit, and SearchResult.

#### **StringList**

typedef sequence <string> StringList;</string>	
Description:	Used to pass and return a set of strings.

# 2.1.2 StrandType

There is an intrinsic directionality of biological sequence data, which proceeds 5' to 3' for nucleic acids and N-terminal to C-terminal for proteins. For **NucleotideSequences**, **StrandType** provides an indication of whether the **SeqRegion** refers to the original plus-strand, the complementary minus-strand, or both strands of a double-stranded molecule. The **StrandType** values are used in **SeqRegion**.

The following table contains the valid **StrandType** for each type of **BioSequence**.

Table 2-1 Valid StrandTypes

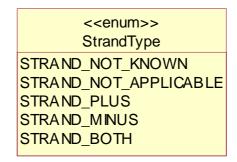
BioSequence Type	Valid StrandTypes
BioSequence	STRAND_NOT_KNOWN
NucleotideSequence	STRAND_NOT_KNOWN, STRAND_PLUS, STRAND_MINUS, STRAND_BOTH
AminoAcidSequence	STRAND_NOT_APPLICABLE

The following table contains the matching **StrandTypes** for each type of **StrandType**.

Table 2-2 Matching StrandTypes

StrandType	Matching StrandTypes
STRAND_NOT_KNOWN	STRAND_NOT_KNOWN, STRAND_PLUS, STRAND_MINUS, STRAND_BOTH
STRAND_NOT_APPLICABLE	STRAND_NOT_APPLICABLE
STRAND_PLUS	STRAND_NOT_KNOWN, STRAND_PLUS, STRAND_BOTH
STRAND_MINUS	STRAND_NOT_KNOWN, STRAND_MINUS, STRAND_BOTH
STRAND_BOTH	STRAND_NOT_KNOWN, STRAND_PLUS, STRAND_MINUS, STRAND_BOTH

2



*Figure 2-1* The StrandType Enumeration.

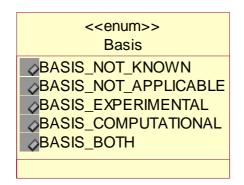
# enum StrandType {STRAND\_NOT\_KNOWN, STRAND\_NOT\_APPLICABLE, STRAND\_PLUS, STRAND\_MINUS, STRAND\_BOTH};

STRAND_NOT_KNOWN	<b>STRAND_NOT_KNOWN</b> should be used in all cases not indicated below.
STRAND_NOT_APPLICABLE	STRAND_NOT_APPLICABLE should be used for regions of AminoAcidSequences.
STRAND_PLUS	<b>STRAND_PLUS</b> should be used to indicate the original plus-strand of a <b>NucleotideSequence</b> .
STRAND_MINUS	<b>STRAND_MINUS</b> should be used to indicate the reverse complement of the plus-strand of a <b>NucleotideSequence</b> .
STRAND_BOTH	<b>STRAND_BOTH</b> should be used to indicate both strands of a double-stranded <b>NucleotideSequence</b> .

# 2.1.3 Basis

The **Basis** enumeration values are used to specify whether an **Annotation** originated from an experimental result or a computational analysis, such as from the application of a sequence analysis program.

2



*Figure 2-2* The Basis Enumeration

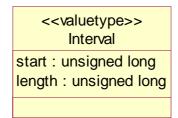
#### enum Basis {BASIS\_NOT\_KNOWN, BASIS\_NOT\_APPLICABLE, BASIS\_EXPERIMENTAL, BASIS\_COMPUTATIONAL, BASIS\_BOTH};

BASIS_NOT_KNOWN	<b>BASIS_NOT_KNOWN</b> should be used in all cases not indicated below.
BASIS_NOT_APPLICABLE	<b>BASIS_NOT_APPLICABLE</b> should be used to indicate that <b>Basis</b> doesn't apply.
BASIS_EXPERIMENTAL	<b>BASIS_EXPERIMENTAL</b> should be used to indicate an experimental result.
BASIS_COMPUTATIONAL	<b>BASIS_COMPUTATIONAL</b> is used to indicate a computational analysis, such as from the application of a sequence analysis program.
BASIS_BOTH	Any result determined both experimentally and computationally should use <b>BASIS_BOTH</b> .

# 2.1.4 Interval

A contiguous sub-string within a larger string is specified using the **Interval** valuetype. An **Interval** consists of a start and length, defining the starting position of the sub-string and the size of the sub-string (number of units). **BioSequences** are numbered starting at start 1, in keeping with the existing practice in the field of molecular biology. An **Interval** on a **BioSequence** of start=5, length=10 would start at the fifth position and include up to the 14th position of a sequence.

The use of a **start** and **length** instead of start and end provides a powerful mechanism for defining intervals along biological sequences that works well for both linear and circular molecules.



*Figure 2-3* The Interval valuetype

#### valuetype Interval

{ public unsigned long start; public unsigned long length;

};

public unsigned long start;	
Description:	<b>start</b> is an unsigned long integer that defines the starting position of the sub-string. <b>BioSequences</b> are numbered starting at 1.
Return value: Returns an <b>unsigned long</b> .	

public unsigned long length;	
Description:	<b>length</b> is an unsigned long integer that defines the size of the sub-string (number of units).
Return value:	Returns an <b>unsigned long</b> .

# 2.1.5 SeqRegion

A SeqRegion is a specialization of Interval and specifies a location on a **BioSequence**. A further specialization, **CompositeSeqRegion**, may contain zero or more sub-regions. In this specification, **SeqRegion** is used primarily to specify the location along a **BioSequence** to which a **SeqAnnotation** pertains.

The **SeqRegion** model is not intended to address all types of sequence region specification found in the GenBank/EMBL/DDBJ feature table. Supported are intervals with non-fuzzy end points and composites of such intervals. Examples of these include a PROSITE pattern located at 74 and ending at 80, or a gene made of 5 spliced exons.

We believe the definition of **SeqRegion** is broad enough to handle many kinds of commonly occurring sequence-based regions and addresses the needs of most molecular biologists. Due to their complexity and rarity of usage in sequence analysis software, fuzzy sequence regions are not explicitly supported at the present time. It is not currently possible with the present IDL to associate a single **SeqRegion** with a set of **BioSequences**.

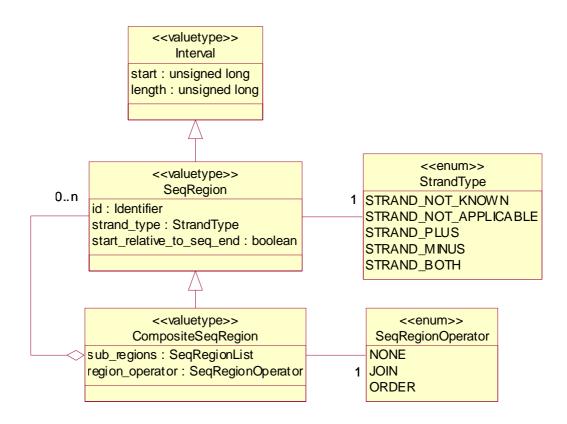


Figure 2-4 The SeqRegion and CompositeSeqRegion Valuetypes

#### SeqRegion

I

A SeqRegion extends Interval and contains the strand\_type and start\_relative\_to\_seq\_end members that specialize it for use with biological sequences. SeqRegion also contains an id indicating the BioSequence to which the SeqRegion refers.

```
valuetype SeqRegion : Interval
{
    public Identifier id;
    public StrandType strand_type;
    public boolean start_relative_to_seq_end;
};
```

public Identifier id;	
Description:	<b>id</b> indicates the <b>BioSequences</b> to which the <b>SeqRegion</b> refers.
Return value:	Returns an <b>Identifier</b> .

public StrandType strand_type;	
Description:	For NucleotideSequences, strand_type provides an indication of whether the SeqRegion refers to the original plus-strand, the complementary minus-strand, or both strands of a double-stranded molecule. STRAND_MINUS should be used to indicate a region on the reverse complement of a NucleotideSequence. For these regions, start and length (inherited from Interval) refer to positions within the coordinate system of the original, given strand. strand_type should be STRAND_NOT_APPLICABLE for regions of AminoAcidSequences.
Return value:	Returns a StrandType.

public boolean start_relative_to_seq_end;	
Description:	The start_relative_to_seq_end member can modify the semantics of the start member: if start_relative_to_seq_end is TRUE, start is to be taken from the end of the sequence, rather than the beginning. No reverse-complement is implied. That is, if sequence has a length 100, and SeqRegion has start=20 length=10, and start_relative_to_seq_end =TRUE, the region runs from position 81 up to and including 90.
Return value:	Returns a <b>boolean</b> .

I

I

I

I

#### **SeqRegionList**

typedef sequence	<seqregion> SeqRegionList;</seqregion>
Description:	Used to pass a set of <b>SeqRegions</b> .

#### **CompositeSeqRegion**

**CompositeSeqRegion**, a specialization of **SeqRegion**, may contain zero or more sub-regions. A **CompositeSeqRegion**'s sub-regions may overlap. The nested or hierarchical behavior is useful in describing complex features on **BioSequences**. There is no limit to nesting. All **CompositeSeqRegions** are expected to be translated in a depth-first traversal, along each node of the tree represented by the **CompositeSeqRegions**. This includes those nodes that have **region\_operator** equal to **JOIN** or **ORDER**.

A **CompositeSeqRegion** with sub-regions will itself not have **start**, **length**, **strand\_type**, or **start\_relative\_to\_seq\_end** data defined. The whole **CompositeSeqRegion** tree will be passed as an object graph by the objects by value (OBV) functionality.

#### valuetype CompositeSeqRegion : SeqRegion

NONE,	// Region has no sub regions or the sub region
	<pre>// don't need special treatment.</pre>
JOIN,	// Sub regions should be joined end-to-end to
	// form a contiguous region.
ORDER	// Sub region order is important.

public SeqRegionOperator region\_operator;

};

I

{

enum SeqRegion	enum SeqRegionOperator {NONE, JOIN, ORDER};	
NONE	<b>NONE</b> should be used when <b>JOIN</b> and <b>ORDER</b> are not applicable.	
JOIN	<b>JOIN</b> should be used when the sub-regions are to be concatenated into a single region.	
ORDER	<b>ORDER</b> should be used when the sub-regions are to be taken as an ordered set of sub-regions. Typically, it is used to represent a discontinuous region to which a descriptive annotation pertains.	

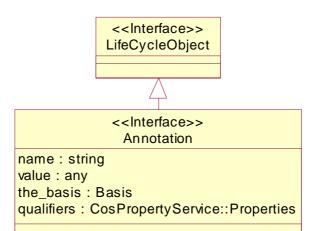
public SeqRegionList sub_regions;	
Description:	<b>sub_regions</b> contains the constituent <b>SeqRegions</b> . If there are no sub-regions, then <b>SeqRegion</b> should be used instead of <b>CompositeSeqRegion</b> .
Return value:	Returns a SeqRegionList.

public SeqRegion	Operator region_operator;
Description:	The <b>region_operator</b> takes on a value of the <b>SeqRegionOperator</b> enumeration. It specifies how the sub- regions are to be treated. The sub-regions could be concatenated into a single region ( <b>JOIN</b> ) or taken as an ordered set of sub-regions ( <b>ORDER</b> ). In the latter case, unknown segments of sequence may intervene. All <b>CompositeSeqRegions</b> are expected to be translated in a depth-first traversal, along each node of the tree represented by the <b>CompositeSeqRegions</b> . This includes those nodes that have <b>region_operator</b> equal to <b>JOIN</b> or <b>ORDER</b> .
Return value:	Returns a SeqRegionOperator.

# 2.1.6 Annotation

The **Annotation** interface defines an annotation that could, in principle, be associated with any bio-object that requires description using name-value pairs.

All attributes in **Annotations** are readonly, in keeping with our immutability policy for this specification.



#### Annotation inherits from CosLifeCycle::LifeCycleObject.

*Figure 2-5* The Annotation Interface

**};** 

I

interface Annotation : CosLifeCycle::LifeCycleObject
{

readonly attribute string name; // type of annotation readonly attribute any value; // the annotation readonly attribute Basis the\_basis; // basis for annotation readonly attribute CosPropertyService::Properties qualifiers;

readonly attribute string name;	
Description:	The <b>name</b> attribute specifies the general type of the annotation that is contained in the value attribute that contains the annotation itself. The value is of type <b>any</b> and therefore could contain anything from a block of free text to a specialized datatype.
Return value:	Returns a <b>string</b> . <b>name</b> shall not be empty.

readonly attribute any value;	
Description:	The <b>value</b> attribute contains the annotation itself.
Return value:	The value is of type <b>any</b> and therefore could contain anything from a block of free text to a specialized datatype.

readonly attribute Basis the_basis;	
Description:	Annotation has a basis attribute, which specifies whether the annotation originated from an experimental result (BASIS_EXPERIMENTAL) or a computational analysis (BASIS_COMPUTATIONAL), such as from the application of a sequence analysis program. Basis provides for a coarse- grained classification of an Annotation.
Return value:	The value is of type <b>BASIS</b> .

readonly attribute CosPropertyService::Properties qualifiers;	
Description:	<ul> <li>Annotation contains additional information in the form of so-called qualifiers, represented by the</li> <li>CosPropertyService::Property struct, which enables them to support many kinds of keyword controlled attributes. These properties are essential for covering the full spectrum of current annotation and feature information.</li> </ul>
Return value:	The <b>qualifiers</b> attribute is of type <b>CosPropertyService::Properties</b> and so provides a place for arbitrary name-value pairs.

# **AnnotationList**

\_\_\_\_\_

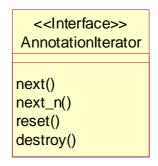
typedef sequence <annotation> AnnotationList;</annotation>	
Description:	Used to pass a set of <b>Annotations</b> .

# **IteratorInvalid**

exception IteratorInvalid { string reason; };	
Description:	The <b>lteratorInvalid</b> exception is raised for cases where the iterator is no longer valid (e.g., new elements have been added to the underlying collection).
Return value:	Returns a <b>string</b> containing the reason that the iterator is invalid.

#### **AnnotationIterator**

AnnotationIterator provides a strongly typed iterator for Annotations.



*Figure 2-6* The AnnotationIterator Interface

#### interface AnnotationIterator

{

{		
-	boolean	next(out Annotation the_annotation)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out AnnotationList annotations)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		

boolean next(out Annotation the_annotation) raises(IteratorInvalid);	
Description:	The <b>next()</b> operation gets the next <b>Annotation</b> in its out parameter <b>the_annotation</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>the_annotation</b> parameter to null.
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>lteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

boolean next_n(in unsigned long how_many, out AnnotationList annotations) raises(IteratorInvalid);	
Description:	<b>next_n()</b> returns <b>Annotations</b> in the <b>AnnotationList</b> out parameter <b>annotations</b> , containing at most the number specified in the first parameter ( <b>how_many</b> ) and returns a boolean value directly. When it is at the end of the set it returns FALSE and the <b>annotations</b> parameter will have length zero. In all cases the length of <b>annotations</b> will be the minimum of <b>how_many</b> and the number of elements remaining.
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>lteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

void reset();	
Description:	<b>reset()</b> sets the iterator to the start of the set.
Exceptions:	Raises CORBA::NO_IMPLEMENT with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).

void destroy();	
Description:	destroy() frees the iterator object.

# 2.1.7 SeqAnnotation

For biomolecular sequences, **Annotations** are specialized to **SeqAnnotations** to include sequence position information in the form of the **SeqRegion** attribute (see above). Essentially, this attribute indicates to which part of the sequence the annotation pertains, and is analogous to features in the DDBJ/EMBL/GenBank formats. Typical examples include gene, promoter region, and exons.

**SeqAnnotation** is used to describe an annotation that applies only to a specified region. **Annotation** should be used for an annotation that applies to the associated **BioSequence** as a whole. Although **SeqAnnotations** with null **regions** are also interpreted to apply to the **BioSequence** as a whole, this should be avoided. **SeqAnnotation** can associate a BioSequence with analytical results or descriptive information such as biological function. A sequence analysis run could generate **SeqAnnotation** objects as output. In addition, **BioSequence** factories can be used to attach **SeqAnnotations** to the **BioSequences**.

It is not currently possible to navigate from a **SeqAnnotation** to a **BioSequence** using the interfaces defined in this specification. One can, however, obtain a set of **SeqAnnotations** given a **BioSequence**. This is sufficient from the point of view of a sequence analysis application, which could produce annotated sequences. The submitters of this specification feel that there are richer models for annotations on sequences (e.g., complex hierarchies or graphs of relationships between annotations and sequences as well as the annotations themselves). Sequence annotations are expected to be addressed in a future RFP.

To illustrate the uses and coverage of **Annotations** and **SeqAnnotations** with regard to the results of Sequence Analyses, a few more examples are listed below:

- A motif analysis returns a labeled pattern (e.g., KRINGLE) matching a given region of the protein sequence.
- A restriction map analysis returns a list of sites, for the given enzymes, that can then be used to annotate the DNA sequence.
- The result of homology analysis suggests that the sequence belongs to a particular gene family, which can be annotated onto the **NucleotideSequence** including information regarding degree of certainty.
- ORF and gene-finding analyses identify coding regions that are later added as oriented gene features on the sequence.
- Homologous regions found by using an alignment analysis can be annotated as **SeqAnnotations** on the query sequence.
- An EMBL-curated phosphorylation site on a protein stored (imported) as a **SeqAnnotation** on the **AminoAcidSequence**.
- Identified mutations from multiple DNA sequences can be merged into **SeqAnnotations** on a consensus sequence.

Extending **SeqAnnotation** provides a mechanism for creating strongly typed sequence features. This may be appropriate for certain stereotypical sequence features such as genes, exons, and transcriptional regulatory sites that have complex but reasonably well defined semantics. These specialized **SeqAnnotations** could define the necessary data types and sub-feature containment relationships as appropriate for the specific feature.

The issue of annotating **BioSequences** as well as other bio-objects is complex and we are not proposing a definitive solution in the present specification. The proposed IDL is workable for biomolecular sequence analysis and there is sufficient room for elaboration by a future LSR Annotation RFP.

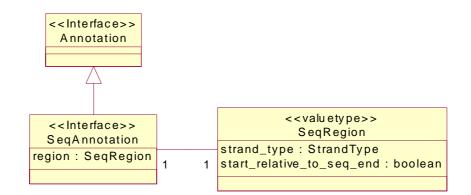


Figure 2-7 The SeqAnnotation Interface

# 2.1.7.1 SeqAnnotation Interface

For biomolecular sequences, **Annotations** are specialized to **SeqAnnotations** to include sequence position information in the form of the **SeqRegion** attribute (see above). If **region** is null, the annotation applies to the associated **BioSequence**(s) as a whole. Otherwise, the annotation applies only to the specified region. **Annotations** should be used instead of **SeqAnnotations** with null **SeqRegions**.

#### interface SeqAnnotation : Annotation

{

readonly attribute SeqRegion seq\_region;

};

readonly attribute SeqRegion seq_region;	
Description:	Contains the sequence position information.
Return value:	Returns a SeqRegion.

### SeqAnnotationList [Variable]

typedef sequence <seqannotation> SeqAnnotationList;</seqannotation>	
Description:	Used to pass a set of <b>SeqAnnotations</b> .

### SeqAnnotationIterator

**SeqAnnotationIterator** provides a strongly typed iterator for **SeqAnnotations**. **SeqAnnotationIterator** is not used directly in this specification, but is provided as a convenience for vendor-specific IDL extensions and future OMG specifications where a collection of **Annotations** contains only **SeqAnnotations**.

SeqAnnotationIterator is an optional interface.

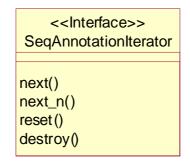


Figure 2-8 The SeqAnnotationIterator Interface

# interface SeqAnnotationIterator

I

{		
•	boolean	next(out SeqAnnotation seq_annotation)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out SeqAnnotationList seq_annotations)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		

boolean next(out SeqAnnotation seq_annotation) raises(IteratorInvalid);	
Description:	The <b>next()</b> operation gets the next <b>SeqAnnotation</b> in its out parameter <b>seq_annotation</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>seq_annotation</b> parameter to null.
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>lteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

boolean next_n(in unsigned long how_many, out SeqAnnotationList seq_annotations) raises(IteratorInvalid);		
Description:	<pre>next_n() returns SeqAnnotations in the SeqAnnotationList out parameter seq_annotations, containing at most the number specified in the first parameter (how_many) and returns a boolean value directly. When it is at the end of the set it returns FALSE and the seq_annotations parameter will have length zero. In all cases the length of seq_annotations will be the minimum of how_many and the number of elements remaining.</pre>	
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>lteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

void reset();	
Description:	reset() sets the iterator to the start of the set.
Exceptions:	Raises CORBA::NO_IMPLEMENT with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).

void destroy();	
Description:	destroy() frees the iterator object.

# 2.1.8 Identifier

There is a need for a data type to indicate an entity's identity in very many situations. In most cases, this need is, or can be addressed by using a string type. The advantages are that it is simple, lightweight, and used universally throughout the realm of computing (and indeed outside). However, the risk of using strings is that they can be too flexible, both in terms of syntax and semantics. This easily results in the lack of interoperability. To allow strings, yet mitigate their potential for abuse, this standard uses the syntax convention of **CosNaming::StringName** as described in the Interoperable Naming service. This convention is mainly a syntactical one; in no way is the use of a naming service implementation required or implied (but it is not precluded either).

# 2.1.8.1 Identifier Description

A brief description is as follows: **CosNaming::Name** is a list of struct **NameComponents**. (For the purpose of illustration, a **NameComponent** can likened to a directory or filename, whereas **CosNaming::Name** constitutes a full path-name). The struct **NameComponent** has string members id and kind. To transform a **CosNaming::Name** into a string, all its **NameComponents** are represented as strings *"id.kind."* 

- If the kind-field is empty, this becomes simply "id;"
- if the id-field is empty, this becomes ".kind;"
- finally, the Naming service allows both id and kind to be empty, which is represented as ".".

The full stringified **CosNaming::Name** is obtained by concatenating all the **NameComponents** using "/" as a separator character. The character "\" is designated as an escape character; if it precedes any of the special characters ".", "/" and "\", they are taken as literal characters. The typedef string **CosNaming::StringName** is provided for strings used as object names using this convention.

This specification adopts this syntax convention, but requests that the components of the **Identifier** data type adhere to some additional semantic constraints. These rules do not follow from, nor are implied by any semantics of the Naming Service. The additional constraints make this data type sufficiently different from **CosNaming::StringName** to warrant the dedicated typedef string **Identifier**.

typedef string Identifier;		
Description:	In this description, 'component' means: the sub-string of an <b>Identifier</b> that corresponds to one <b>CosNaming::NameComponent</b> ; likewise, id-field and kind-field correspond to the equivalent fields of <b>NameComponent</b> .	

The rules are as follows:

- Names can refer to collections of entities (such as databases), or to entities within such collections. Names referring to collections consist of exactly one component; names referring to entities within collections consist of at least two components.
- The first component represents the data source. Data sources can be anything: transient collections, local databases, public repositories. It is up to the implementation to document the accepted names for the data source.
- The empty name (".") is valid for the first component, and represents the 'local' or 'default' collection. It is up to the implementation to document what the semantics of 'local' or 'default' is.

- Names that refer to entities within collections consist of two or more components. The second component of such names represents an identifier that is unique in the context of the data source. No empty id-fields are allowed in this or any further components.
- If two components are not enough to uniquely identify an entity, an Identifier can contain more than two components, but no more than necessary to make the identification unique. That is, an Identifier may not be used to freely attach textual information.
- The only characters valid in a component are "a" through "z", "0" through "9", and "-" (hyphen), "\_" (underscore), "\$" and "." (period). Use of the latter is discouraged since it has a special meaning in the stringifying convention, and has therefore to be escaped.
- To comply with existing practice in the field of public data repositories, it is strongly advised that implementations do string comparisons in a case-insensitive manner. The Naming Service standard fails to mention whether type-case is, for identification purposes, significant or not. Implementations that use a third-party implementation of the Naming Service may therefore wish to restrict Identifiers to only use one type-case. It is up to an implementation to state whether mixed type-case is allowed, and whether type-case is significant in comparisons.

The *id* and *kind* parts of the string components of **Identifier** are used as follows:

- The id-field of a component contains the principal value that makes it unique in the scope provided by the preceding component. It may only be empty in the case of the first component of an Identifier.
- The kind-field of a component is used to represent information indicating the release (for a data source) or version (for an entry) of an entity, and can be empty. If kind is empty and entities with non-empty kind-fields exist, an empty kind field becomes synonymous with the latest release or version. It is up to the implementation to document the syntax and semantics of the version information.

The adoption of this convention has the following advantages:

- it is simple and lightweight,
- it has a well-defined and re-used syntax,
- it is compatible with existing practice,
- it is sufficiently flexible to allow for sub-ids if necessary.

# IdentifierList

typedef sequence <identifier> IdentifierList;</identifier>	
Description:	Used to pass a set of <b>Identifiers</b> .

# **IdentifierNotFound**

exception IdentifierNotFound { Identifier id; };	
Description:	The <b>IdentifierNotFound</b> exception is raised for cases where the database and the identifier within the database can be resolved but the Identifier is not present.
Return value:	Returns the <b>Identifier</b> that could not be found.

### IdentifierNotResolvable

exception IdentifierNotResolvable { Identifier id; string reason; };	
Description:	The <b>IdentifierNotResolvable</b> exception is raised for cases where database and the identifier within the database cannot be resolved such that the <b>Identifier</b> cannot even be searched for.
Return value:	Returns the <b>Identifier</b> that could not be resolved and a string containing the reason resolution was not possible.

### IdentifierNotUnique

exception IdentifierNotUnique { Identifier id; IdentifierList ids; };	
Description:	The <b>IdentifierNotUnique</b> exception is raised for cases when the <b>Identifier</b> specification is ambiguous and returns more than one object.
Return value:	Returns the non-unique <b>Identifier</b> and an <b>IdentifierList</b> containing <b>Identifiers</b> for all objects that id identifies.

### 2.1.9 BioSequence

A **BioSequence** is an abstraction of a biological sequence, such as the ordered nucleotides of a DNA chain or the ordered amino acid residues of a protein molecule. A **BioSequence** can be of any length and significance; there is no implication that it corresponds to, for example, a gene. The **BioSequence** interface provides essential characteristics of biological sequences (**name**, **id**, **description**, **length**) and operations for obtaining the sequence string itself or a sub-sequence as an ASCII string of IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) upper case single letter codes (**seq()**, **seq\_interval()**).

Additional operations within **BioSequence** provide access to any annotations associated with the **BioSequence** (get\_annotations()) or the number of annotations (num\_annotations()).

Annotations can be attached to BioSequences directly using the add\_annotation() method of BioSequence or by using the BioSequence factories. Thus, BioSequences are mutable at the level of their associated annotations. This minimal mutability model permits new annotations to be attached to a BioSequence and prevents situations where multiple BioSequences might exist on a server with different sets of annotations but representing the same sequence. A NotUpdateable exception can be used to indicate that an Annotation cannot be added to this BioSequence.

Standard container behavior applies here. If a client destroys a **BioSequence**, it is also up to the client to manage the contents, namely the **Annotations**.

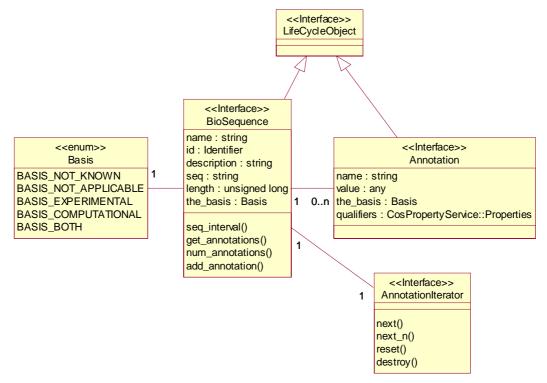


Figure 2-9 The BioSequence Interface

I

### IntervalOutOfBounds

exception IntervalOutOfBounds {     Interval invalid;     Interval valid; };	
Description:	<ul> <li>The IntervalOutOfBounds exception is raised if an</li> <li>Interval's start is less than 1 or if its start+length-1 is</li> <li>greater than the length of the BioSequence. If a</li> <li>BioSequence represents circular DNA, then this exception</li> <li>should be raised if the Interval's start is less than 1 or</li> <li>greater than the length of the BioSequence, or if its length</li> <li>is greater than that of the BioSequence.</li> </ul>
Return value:	Returns the invalid <b>Interval</b> and the valid <b>Interval</b> . The valid <b>Interval</b> has <b>start</b> equal to 1 and <b>length</b> equal to the length of the <b>BioSequence</b> , the largest allowed <b>Interval</b> .

# SeqRegionOutOfBounds

exception SeqRegionOutOfBounds {     SeqRegion invalid;     Interval valid; };	
Description:	The SeqRegionOutOfBounds exception is raised if a SeqRegion's start is less than 1 or if its start+length-1 is greater than the length of the BioSequence. The exception is also raised if a nested sub-region of a CompositeSeqRegion is invalid. If a BioSequence represents circular DNA, then this exception should be raised if the Interval's start is less than 1 or greater than the length of the BioSequence, or if its length is greater than that of the BioSequence.
Return value:	Returns the invalid <b>SeqRegion</b> and the valid <b>Interval</b> . The valid <b>Interval</b> has <b>start</b> equal to 1 and <b>length</b> equal to the length of the <b>BioSequence</b> , the largest allowed <b>Interval</b> .

### SeqRegionInvalid

exception SeqRegionInvalid { string reason; };	
Description:	The SeqRegionInvalid exception is raised if a SeqRegion or CompositeSeqRegion is invalid in a given context. Examples include the StrandType being STRAND_BOTH when trying to translate a nucleotide sequence, or a wrong SeqRegionOperator, overlaps, or circularity in a CompositeSeqRegion passed as an in parameter.
Return value:	Returns a string containing the reason the <b>SeqRegion</b> is invalid.

### NotUpdateable

exception NotUpdateable { string reason; };	
Description:	The NotUpdateable exception is raised if the <b>BioSequence</b> is immutable.
Return value:	Returns a string containing the reason the <b>BioSequence</b> cannot be updated.

#### BioSequence

A **BioSequence** is an abstraction of a biological sequence, such as the ordered nucleotides of a DNA chain or the ordered amino acid residues of a protein molecule. The **BioSequence** interface provides essential characteristics of biological sequences (**name**, **id**, **description**, **length**) and operations for obtaining the sequence string itself or a sub-sequence as an ASCII string of IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) upper case single letter codes (**seq(**), **seq\_interval(**)).

BioSequence inherits from CosLifeCycle::LifeCycleObject.

interface BioSequence : CosLifeCycle::LifeCycleObject

{

readonly attribute string readonly attribute Identifier readonly attribute string readonly attribute string readonly attribute unsigned long readonly attribute Basis

name; id; description; seq; length; the\_basis;

string

seq\_interval(in Interval the\_interval)

raises(IntervalOutOfBounds, SeqRegionInvalid);
get_annotations(
in unsigned long how_many,
in SeqRegion seq_region,
out AnnotationIterator the_rest)
raises(SeqRegionOutOfBounds, SeqRegionInvalid);
num_annotations(in SeqRegion seq_region)
raises(SeqRegionOutOfBounds, SeqRegionInvalid);
add_annotation(
in Annotation the_annotation)
raises(NotUpdateable, SeqRegionOutOfBounds,
SeqRegionInvalid);

I

I

};

readonly attribute string name;	
Description:	The <b>name</b> attribute represents a human-readable common name for the <b>BioSequence</b> (such as a gene name).
Return value:	Returns a string.

readonly attribute Identifier id;	
Description:	The <b>id</b> attribute represents an ID for the <b>BioSequence</b> . Typically a database name and key will be encoded in the <b>Identifier</b> .
Return value:	Returns an <b>Identifier</b> . <b>id</b> shall not be empty

readonly attribute string description;	
Description:	The <b>description</b> attribute, a concise description of the <b>BioSequence</b> , typically includes functional information, e.g., the contents of the description line from a FASTA file.
Return value:	Returns a string.

readonly attribute string seq;	
Description:	The <b>seq</b> attribute contains the actual sequence data. The entire sequence is returned. Use <b>seq_interval()</b> to access sub-sequences.
Return value:	Returns an ASCII string of IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) upper case single letter codes representing the entire sequence. The string will not contain any termination characters (e.g., '*') or gap characters (e.g., '-').

readonly attribute unsigned long length;	
Description:	The <b>length</b> attribute is the length of the <b>BioSequence</b> . The <b>BioSequence</b> is numbered from 1 to <b>length</b> .
Return value:	Returns an unsigned long.

readonly attribute Basis the_basis;	
Description:	The <b>BioSequence basis</b> attribute can be any of the values of the <b>Basis</b> enumeration and specifies whether the sequence has been experimentally determined ( <b>BASIS_EXPERIMENTAL</b> ), computationally determined ( <b>BASIS_COMPUTATIONAL</b> ), or both ( <b>BASIS_BOTH</b> ), or if this information is not known ( <b>BASIS_NOT_KNOWN</b> ). An example of a computational sequence would be a protein sequence that was determined by in silico translation of an
	experimentally determined DNA sequence.
Return value:	Returns a <b>Basis</b> value.

\_\_\_\_\_

string seq_interval(in Interval the_interval) raises(IntervalOutOfBounds, SeqRegionInvalid);	
Description:	Provides access to sub-sequences of the <b>BioSequence</b> . The Interval argument indicates which sub-sequence should be returned. The entire sequence may also be obtained using the <b>seq</b> attribute. If the_interval is a <b>SeqRegion</b> and the <b>StrandType</b> is <b>STRAND_MINUS</b> , the string returned should be taken as reverse- complemented.
Return value:	Returns an ASCII string of IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) upper case single letter codes representing the appropriate sub-sequence.
Exceptions:	<ul> <li>Raises IntervalOutOfBounds if the Interval's start is less than 1 or if its start+length-1 is greater than the length of the BioSequence. If the BioSequence represents circular DNA, then this exception should be raised if the Interval's start is less than 1 or greater than the length of the BioSequence, or if its length is greater than that of the BioSequence.</li> <li>Raises SeqRegionInvalid if the_interval is a invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).</li> </ul>

I

I

AnnotationList get_annotations( in unsigned long how_many, in SeqRegion seq_region, out AnnotationIterator the_rest) raises(SeqRegionOutOfBounds, SeqRegionInvalid);	
Description:	Uses the list/iterator hybrid to provide access to the <b>Annotations</b> . A list of no more than <b>how_many</b> elements is returned as the direct result. The remaining elements, if any, are available through the iterator returned in the <b>out</b> parameter. Only the <b>SeqAnnotations</b> that overlap <b>seq_region</b> and have compatible <b>StrandTypes</b> will be returned. If <b>seq_region</b> is null, only <b>Annotations</b> are returned.

...continued

Return value:	Returns an <b>AnnotationList</b> containing no more than <b>how_many</b> elements. The <b>AnnotationIterator</b> provides access to any remaining elements.
Exceptions:	Raises SeqRegionOutOfBounds if seq_region is out of bounds for this BioSequence. Raises SeqRegionInvalid if the SeqRegion is invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

unsigned long num_annotations(in SeqRegion seq_region) raises(SeqRegionOutOfBounds, SeqRegionInvalid);	
Description:	Provides access to the number of <b>Annotations</b> associated with this <b>BioSequence</b> . Only the <b>SeqAnnotations</b> that overlap <b>seq_region</b> and have compatible <b>StrandTypes</b> will be counted. If <b>seq_region</b> is null, only <b>Annotations</b> are counted.
Return value:	Returns an unsigned long.
Exceptions:	Raises SeqRegionOutOfBounds if seq_region is out of bounds for this BioSequence.
	Raises SeqRegionInvalid if the SeqRegion is invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

I

void add_annotation(in Annotation the_annotation) raises(NotUpdateable, SeqRegionOutOfBounds, SeqRegionInvalid);	
Description:	Annotations can be attached to <b>BioSequences</b> directly using the <b>add_annotation()</b> method of <b>BioSequence</b> .
Exceptions:	Raises NotUpdateable if the <b>BioSequence</b> is immutable. Raises SeqRegionOutOfBounds if the <b>Annotation</b> is a <b>SeqAnnotation</b> and the corresponding <b>SeqRegion</b> is out of bounds for this <b>BioSequence</b> .
	Raises SeqRegionInvalid if the Annotation is a SeqAnnotation that has a SeqRegion that is deemed invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

#### **BioSequenceList**

typedef sequence <biosequence> BioSequenceList;</biosequence>	
Description:	Used to pass a set of <b>BioSequences</b> .

# 2.1.10 Sub-types of BioSequence

I

The data type **BioSequence** is an interface representing biological sequences. All instances of actual biological sequences are expected to derive from one of the **BioSequence** sub-types, **NucleotideSequence** or **AminoAcidSequence** (or specialized sub-types thereof).

Sequence information input to a **BioSequence** or used for querying purposes is caseinsensitive. Sequence information output from a **BioSequence** is returned using uppercase ASCII strings of IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single-letter character codes.

**AminoAcidSequence** represents a protein sequence and does not contain any operations. A reverse translation operation that produces a nucleic acid sequence from the amino acid sequence is a complex operation that is not straightforward to standardize at this time.

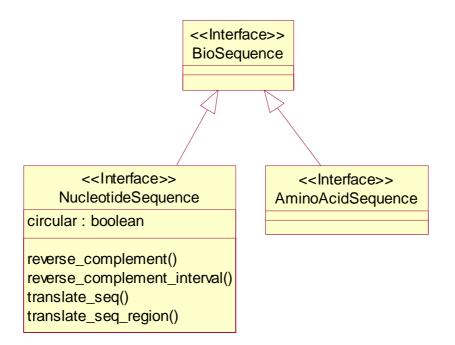


Figure 2-10 The NucleotideSequence and AminoAcidSequence Interfaces

### **UnsignedLongList**

typedef sequence <unsigned long=""> UnsignedLongList;</unsigned>	
Description:	Used to pass a set of <b>unsigned longs</b> .

#### **Reading Frame Invalid**

exception ReadingFrameInvalid { short invalid; };	
Description:	The <b>ReadingFrameInvalid</b> exception is raised if the reading frame is not between -3 and +3, excluding zero.
Return value:	Returns a <b>short</b> containing the invalid reading frame.

### NucleotideSequence

{

**NucleotideSequence** extends **BioSequence** and represents a DNA or RNA sequence and provides a number of operations for manipulating the sequence data. There is an intrinsic directionality of nucleotide sequence data, from 5' to 3'.

### interface NucleotideSequence : BioSequence

readonly attribute boolean circular;

string	reverse_complement();
string	reverse_complement_interval(in Interval the_interval) raises(IntervalOutOfBounds, SeqRegionInvalid);
string	translate_seq( in short reading_frame, out UnsignedLongList stop_locations) raises(ReadingFrameInvalid);
string	translate_seq_region( in SeqRegion seq_region, out UnsignedLongList stop_locations) raises(SeqRegionOutOfBounds, SeqRegionInvalid);

};

readonly attribute boolean circular;	
Description:	The <b>circular</b> attribute provides a mechanism to indicate whether a <b>NucleotideSequence</b> is circular, as is the case for plasmids or certain microbial chromosomes.
Return value:	Returns a TRUE if the <b>NucleotideSequence</b> is circular and FALSE otherwise.

string reverse_complement();	
Description:	<b>reverse_complement()</b> returns an upper-case ASCII string consisting of the reverse complement of the given <b>NucleotideSequence</b> .
Return value:	Returns an upper-case ASCII string.

string reverse_complement_interval(in Interval the_interval) raises(IntervalOutOfBounds);	
Description:	reverse_complement_interval() permits the retrieval of a
	reverse complement string for a sub-sequence of the given sequence defined by the <b>Interval</b> argument. If <b>the_interval</b> is a <b>SeqRegion</b> and the <b>StrandType</b> is <b>STRAND_MINUS</b> , the string returned should be taken as reverse-complemented. This
	will result in a no-op (i.e., the <b>strand_type</b> leads to reverse- complementing), which is then reverse-complementing due to the semantics of the method, resulting in the same string that would be returned from <b>seq_interval</b> ().

...continued

Return value:	Returns an upper-case ASCII string.
Exceptions:	Raises IntervalOutOfBounds if the Interval's start is less than 1 or its start+length-1 is greater than the length of the NucleotideSequence. If the NucleotideSequence represents circular DNA, then this exception should be raised if the Interval's start is less than 1 or greater than the length of the NucleotideSequence, or if its length is greater than that of the NucleotideSequence.
	Raises SeqRegionInvalid if the_interval is an invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

string translate_seq( in short reading_frame, out UnsignedLongList stop_locations) raises(ReadingFrameInvalid);	
Description:	<ul> <li>translate_seq() returns a string representing the conceptual amino acid translation of the nucleic acid sequence.</li> <li>translate_seq() requires the reading frame in which the translation is to be performed. The reading_frame should be a signed integer (short) between -3 and +3, excluding zero. If reading_frame is positive, (reading_frame - 1) nucleotides at the beginning (5' end) of the sequence are ignored. If reading_frame is negative, its absolute value should be applied to the 5' end of the complementary (minus) strand.</li> </ul>
Return value:	The returned <b>string</b> consists of upper-case single-letter IUPAC- IUBMB Joint Commission on Biochemical Nomenclature (JCBN) character codes for the translated amino acids. Any internal stop codons are represented by '*'. The <b>UnsignedLongList out</b> parameter <b>stop_locations</b> contains the locations of any internal stops (terminators) in the protein translation.
Exceptions:	Raises ReadingFrameInvalid if reading_frame is not between -3 and +3, excluding zero.

string translate_seq_region( in SeqRegion seq_region, out UnsignedLongList stop_locations) raises(SeqRegionOutOfBounds, SeqRegionInvalid);	
Description:	<ul> <li>translate_seq_region() performs a translation of a defined region of a NucleotideSequence specified by the SeqRegion argument. No reading frame is necessary because the SeqRegion defines the frame. A SeqRegion is required here instead of an interval because non-contiguous segments of a NucleotideSequence may need to be specified, as in the case of a DNA sequence containing introns. If a region submitted for translation contains sub-regions, all sub-regions are concatenated in depth-first order prior to translation. If seq-region's StrandType is STRAND_MINUS, the string returned should be taken as reverse-complemented before being translated.</li> </ul>
Return value:	The returned <b>string</b> consists of upper-case single-letter IUPAC- IUBMB Joint Commission on Biochemical Nomenclature (JCBN) character codes for the translated amino acids. Any internal stop codons are represented by '*'. The <b>UnsignedLongList out</b> parameter <b>stop_locations</b> contains the locations of any internal stops (terminators) in the protein translation.
Exceptions:	Raises SeqRegionOutOfBounds if any contained Interval's start is less than 1 or its start+length-1 is greater than the length of the NucleotideSequence. If the NucleotideSequence represents circular DNA, then this exception should be raised if the SeqRegion's start is less than 1 or greater than the length of the NucleotideSequence, or if its length is greater than that of the NucleotideSequence.         Raises SeqRegionInvalid if seq_region is invalid. Examples include an incorrect StrandType, or an invalid         CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

### *NucleotideSequenceList*

<pre>typedef sequence<nucleotidesequence> NucleotideSequenceList;</nucleotidesequence></pre>	
Description:	Used to pass a set of NucleotideSequences.

#### *AminoAcidSequence*

**AminoAcidSequence** extends **BioSequence** and represents a protein sequence and does not contain any operations. A reverse translation operation that produces a nucleic acid sequence from the amino acid sequence is a complex operation that is not straightforward to standardize at this time. There is an intrinsic directionality of protein sequence data, from N-terminal to C-terminal.

#### interface AminoAcidSequence : BioSequence

{ };

*AminoAcidSequenceList* 

<pre>typedef sequence<aminoacidsequence> AminoAcidSequenceList;</aminoacidsequence></pre>	
Description:	Used to pass a set of AminoAcidSequences.

### 2.1.11 CodeRule

**CodeRule** is a valuetype that defines the correspondence between a **Codon** and a **Residue** type. The **Residue** member (residue) is a single ASCII character representing an amino acid in the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) standard. The **Codon** member (codon) is an array of three **Bases**, which are characters representing unambiguous nucleotides using the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for nucleotide nomenclature (see References).

#### Residue

typedef char	Re	sidue;
Description:		The <b>Residue</b> member (residue) is a single ASCII character representing an amino acid using the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for amino acid nomenclature (see References).

### Base

typedef char Base;	
Description:	A <b>Base</b> is a character representing an unambiguous nucleotide using the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for nucleotide nomenclature (see References).

### Codon

typedef Base	Codon[3];	
Description:	A Codon is an array of three Bases.	

### CodeRule

**CodeRule** is a valuetype that defines the correspondence between a **Codon** and a **Residue** type.

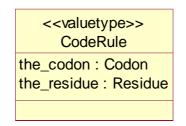


Figure 2-11 The CodeRule valuetype

### valuetype CodeRule

{
 public Codon the\_codon;
 public Residuethe\_residue;
};

public Codon the_codon;	
Description:	The <b>Codon</b> member (codon) is an array of three <b>Bases</b> , which are characters representing unambiguous nucleotides using the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for nucleotide nomenclature (see References).
Return value:	Returns a <b>Codon</b> .

public Residue the_residue;	
Description:	The <b>Residue</b> member (residue) is a single ASCII character representing an amino acid using the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for amino acid nomenclature (see References).
Return value:	Returns a <b>Residue</b> .

# Coding

\_\_\_\_\_

typedef CodeRule Coding[64];	
Description:	A <b>Coding</b> is an array of sixty-four <b>CodeRules</b> . Sixty-four is the number of combinations of the four <b>Bases</b> (A, G, C, U) taken three at a time.

### GeneticCodeName

typedef string	GeneticCodeName;	
Description:	A <b>GeneticCodeName</b> is a <b>string</b> that contains the name of a currently known genetic code.	
	a currently known genetic code.	

# GeneticCodeNameList

typedef sequence <geneticcodename> GeneticCodeNameList;</geneticcodename>	
Description:	Used to pass a set of GeneticCodeNames.

### InvalidResidue

<pre>exception InvalidResidue {     Residue the_residue;     unsigned long offset; };</pre>	
Description:	The InvalidResidue exception is raised if the <b>Residue</b> is inconsistent with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes. Note that residue may be interpreted to mean base (see Glossary).
Return value:	Returns the invalid <b>Residue</b> and its offset within the <b>BioSequence</b> .

# 2.1.12 GeneticCode

I

The GeneticCodeFactory interface defines a set of const GeneticCodeName strings that list the set of currently known genetic codes. A GeneticCode object should be created with its name member set to one of these GeneticCodeNames. The GeneticCode object is used for translating a string of nucleic acid bases into a string of amino acid residues. The GeneticCodeName defines the particular Coding that is used to convert Codons into Residues so one need only specify the GeneticCodeName when creating a GeneticCode object from one of the known types. Codings for the GeneticCodeNames listed below in GeneticCodeFactory can be found in Appendix B "Genetic Codes".

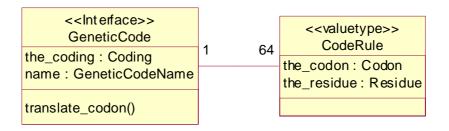


Figure 2-12 The GeneticCode interface

interface GeneticCode : CosLifeCycle::LifeCycleObject
{
 readonly attribute Coding the\_coding;
 readonly attribute GeneticCodeName name;

```
Residue translate_codon(in Codon the_codon) raises(InvalidResidue);
```

};

readonly attribute Coding the_coding;	
Description:	The <b>coding</b> attribute consists of an array of 64 <b>CodeRules</b> , which allows the <b>GeneticCode</b> object to be used for translating a string of nucleic acid bases into a string of amino acid residues. <b>Codings</b> for the <b>GeneticCodeNames</b> listed below in <b>GeneticCodeFactory</b> can be found in Appendix B.
Return value:	Returns a <b>Coding</b> .

readonly attribute GeneticCodeName name;	
Description:	The <b>name</b> attribute should be one of the known <b>GeneticCodeNames</b> listed in <b>GeneticCodeFactory</b> . If the desired genetic code is not represented, an appropriate name should be used.
Return value:	Returns a GeneticCodeName.

Residue translate_codon(in Codon the_codon) raises(InvalidResidue);	
Description:	<b>translate_codon</b> () uses <b>coding's</b> array of sixty-four <b>CodeRules</b> to translate a string of nucleic acid bases into a string of amino acid residues.
Return value:	Returns a <b>Residue</b> .
Exceptions:	Raises InvalidResidue if the codon is inconsistent with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes. Note that residue is interpreted to mean base here (see Glossary).

# 2.1.13 AlignmentElement

An **AlignmentElement** corresponds to one 'row' in a traditional alignment. However to make it general, it is represented by a wrapper that allows any **Object** to be used in an **Alignment**. This approach allows the occurrence of one and the same **Object** in different 'rows' (using the **key**), and also avoids the combinatorial problem of having every type of **BioSequence** duplicated just so it can be used in an **Alignment**. This approach allows other objects, not yet defined in this standard (e.g., hidden Markov models, to be used in the alignment). Most commonly, however, **AlignmentElement** will contain an **element** of type **BioSequence**.

The **key** provides a unique reference to each **AlignmentElement** to be maintained between the client and the server of the **Alignment**. Notice that there may be more than one copy of a particular **Object** in the **Alignment**. There is no proscribed semantics to how the **key** is structured. The following provides examples of **keys** that could be used if the **Objects** are **BioSequences**.

Unique BioSequence Identifiers		
Identifiers	Example Key Set 1	Example Key Set 2
emb/X04427	emb/X04427	0
emb/XX1111	emb/XX1111	1

### Table 2-3 Key Examples

1 (3775541	1 1275541	2
emb/X75541	emb/X75541	2
emb/Y10276	emb/Y10276	3
emb/X95248	emb/X95248	4
Non-unique BioSequence	Identifiers (repeated sequen	ice)
	1	,
Identifiers	Example Key Set 1	Example Key Set 2
emb/X04427	emb/X04427	0
emb/XX1111	emb/XX1111	1
emb/X75541	emb/X75541	2
emb/Y10276	emb/Y10276	3
emb/X95248	emb/X95248/0	4
emb/X95248	emb/X95248/1	5

< <valuetype>&gt; AlignmentElement</valuetype>
element : Object seq_region : SeqRegion key : string

Figure 2-13 The AlignmentElement valuetype.

### AlignmentElement

valuetype AlignmentElement

public Objectelement;public SeqRegionseq\_region;public stringkey;

};

public Object element;				
Description:	The analysis that constructs the <b>Alignment</b> is responsible for determining if the <b>Object</b> is appropriate in the given context. Most commonly, <b>AlignmentElement</b> will simply contain an <b>element</b> of type <b>BioSequence</b> .			
Return value:	Returns an <b>Object</b> .			

public SeqRegion seq_region;					
Description:	The <b>seq_region</b> represents the coordinates of a particular segment of the <b>element</b> (typically a <b>BioSequence</b> ) that is aligned in the current <b>Alignment</b> , and that is considered one 'row' in the <b>Alignment</b> . The coordinates are those of the original <b>Object</b> , not those of the <b>Alignment</b> . Notice that a particular <b>Object</b> might be represented more than once in the <b>Alignment</b> , and <b>seq_region</b> will provide the information as to the region of the <b>Object</b> that is used. The only valid <b>SeqRegionOperator</b> is <b>JOIN</b> .				
Return value:	Returns a <b>SeqRegion</b> .				

public string key;	
Description:	The key provides a unique reference to each <b>AlignmentElement</b> to be maintained between the client and the server of the <b>Alignment</b> . Notice that there may be more than one copy of a particular <b>Object</b> in the <b>Alignment</b> . There is no proscribed semantics to how the <b>key</b> is structured. It is used in the <b>get_seq_region()</b> method in <b>Alignment</b> to provide a unique key for this <b>AlignmentElement</b> .
Return value:	Returns a <b>string</b> .

### AlignmentElementList

<pre>typedef sequence<alignmentelement> AlignmentElementList;</alignmentelement></pre>					
Description:	Used to pass a set of AlignmentElements.				

# 2.1.14 AlignmentElementIterator

AlignmentElementIterator provides a strongly typed iterator for AlignmentElements.

< <interface>&gt; AlignmentElementIterator</interface>
next()
next_n()
reset() destroy()

Figure 2-14 The AlignmentElementIterator Interface.

# interface AlignmentElementIterator {

{		
-	boolean	next(out AlignmentElement element)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out AlignmentElementList elements)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		
• •		

boolean next(out AlignmentElement element) raises(IteratorInvalid);					
Description:	The <b>next()</b> operation gets the next <b>AlignmentElement</b> in its out parameter <b>element</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>element</b> parameter to null.				
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.				
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).				

boolean next_n(in unsigned long how_many, out AlignmentElementList elements) raises(IteratorInvalid);					
Description:	<b>next_n()</b> returns <b>AlignmentElements</b> in the <b>AlignmentElementList out</b> parameter <b>elements</b> , containing at most the number specified in the first parameter ( <b>how_many</b> ) and returns a boolean value directly. When it is at the end of the set it returns FALSE and the <b>elements</b> parameter will have length zero. In all cases the length of <b>elements</b> will be the minimum of <b>how_many</b> and the number of elements remaining.				
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.				
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).				

void reset();	
Description:	reset() sets the iterator to the start of the set.
Exceptions:	Raises <b>CORBA</b> :: <b>NO_IMPLEMENT</b> with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).

void destroy();	
Description:	destroy() frees the iterator object.

# 2.1.15 Alignment

An **Alignment** is built from a set of correspondences of regions of sequences. In many cases the sequence region is only a single residue (a single base or a single amino acid) long, but this need not be. For example, a region of three DNA base pairs, representing a single amino acid, is a common region size. Each correspondence, which is called a 'column' due to the common visual interpretation of an alignment, indicates that a particular region of one sequence is in some manner equivalent to set of particular regions on other sequences. The exact nature of this equivalence differs between different alignment methods, the most common being that these regions shared a common evolutionary ancestor. An alternative is that these regions were read from the same region of physical DNA, as in a DNA assembly.

Alignment representation in sequence analysis has been dominated by text based representation of the correspondences as columns, with sequences running horizontally and each correspondence being represented by a column. Padding characters (often '-') are placed in sequences to align the residues with the correct correspondences in other sequences.

seql	10	RSDGFAFVEF	19
seq2	15	RT-GFAYVEM	23
seq3	20	RTHGFAFVEM	29

Table 2-4 Multiple Alignment of AminoAcidSequences

Correspondence	1:	(Seql,	position	10,	Seq2,	position	15,	Seq3	position	20)
Correspondence	2:	(Seql,	position	11,	Seq2,	position	16,	Seq3	position	21)
Correspondence	3:	(Seql,	position	12,	Seq2,	none,		Seq3	position	22)
Correspondence	10:	(Seql,	position	19,	Seq2,	position	23,	Seq3	position	29)

This provides a compact representation of the alignment, but relies heavily on single characters being the basis of the correspondence, which makes representing more complex but still common types of alignment challenging. Examples include alignments of DNA and protein sequences and alignments of profile Hidden Markov Models and protein sequences. In addition, text based representation cannot convey any additional information about the nature of the correspondence, which is an issue for more complex alignments. A final drawback to this method of representing an alignment is that it is generally hard to examine only part of the alignment, as the entire text must be processed before the correspondences between positions can be represented explicitly in computer terms.

An IDL definition of an alignment can provide a much richer description of an alignment, but it must be kept in mind that the most common use of an alignment will be to view it, probably in a form very close to Table 2-4. Generating a similar text representation must be simple operation for a client of the **Alignment** interface.

For complex alignments it is convenient to associate with each correspondence the assumption on which the correspondence is made. For example, when aligning a protein sequence to a DNA sequence, it is important to be able to distinguish insertions in the DNA sequence which are due to sequencing errors in the determination of the DNA sequence. This implies that each correspondence needs an indication of the assumptions made for the grouping of regions on sequences. Such assumptions are generally made during the alignment process. As such, they are not a fixed property of one particular sequence in the alignment, but they rather belong to the alignment as a whole. Therefore, it is better to associate the assumption(s) with the correspondences, rather than with the sequences.

Although many of the alignments involve **BioSequences**, there are a number which also involve other objects, such as regular expressions and hidden Markov models. These objects are not part of this specification, and, in any case, it is unlikely that any

specification could cover all possible objects that will be designed in this field. The proposed specification can handle any CORBA object through the **AlignmentElement** wrapper.

The proposed **Alignment** interface can model simple and complex alignments in a complete way. The object provides accessors to retrieve all the correspondences and the individual regions inside a correspondence. There is no explicit **correspondence** or **column** object, as it seems of little value. Users will generally be using a set of correspondences (i.e., an alignment).

We recognize that there are many uses of an alignment where the client does not want to process the actual alignment information itself, but simply wants to display it to a user or pass it onto programs which are based around old text based alignment formats. The optional **CharacterAlignmentEncoder** interface provides a way for a client to get a more traditional view of an **Alignment**. In addition, this interface lets the server take responsibility for the representation of an **Alignment**. This way, servers can offer clients a complete solution, including representation. For complex alignments that are non-trivial to render, this is an important mechanism. We cannot stress too highly that the representation of an **Alignment**, especially that of gaps, is the job of the **CharacterAlignmentEncoder** and not that of the corresponding **Alignment**.

### **AlignmentObjectInvalid**

exception AlignmentObjectInvalid {     Object element;     string reason; };	
Description:	The AlignmentObjectInvalid exception is raised if the <b>Object</b> is not valid for this <b>Alignment</b> . This exception will be raised by analyses that construct <b>Alignments</b> .
Return value:	Returns the invalid <b>Object</b> and a <b>string</b> containing the reason the element is invalid.

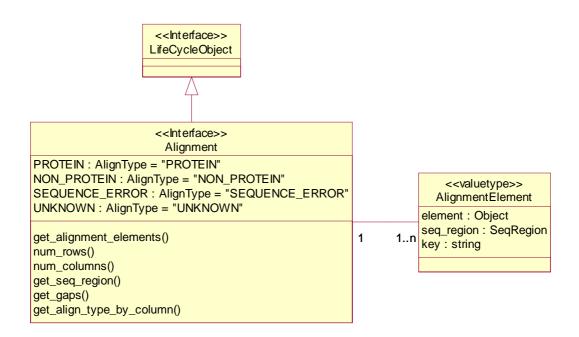
#### *ElementNotInAlignment*

exception ElementNotInAlignment { };	
Description:	The ElementNotInAlignment exception is raised if the <b>AlignmentElement</b> is not associated with this <b>Alignment</b>

### IndexOutOfBounds

exception IndexOutOfBounds {     unsigned long invalid;     Interval valid; };	
Description:	The IndexOutOfBounds exception is raised if an index is out of bounds.
Return value:	Returns the invalid <b>unsigned long</b> and the valid <b>Interval</b> . The valid <b>Interval</b> contains the largest allowed <b>Interval</b> for the index.

#### Alignment





{

interface Alignment : CosLifeCycle::LifeCycleObject

typedef string AlignType; typedef sequence<AlignType> AlignTypeList; const AlignType PROTEIN = "PROTEIN"; const AlignType NON\_PROTEIN = "NON\_PROTEIN"; const AlignType SEQUENCE\_ERROR = "SEQUENCE\_ERROR"; const AlignType UNKNOWN = "UNKNOWN";

AlignmentElementList get\_alignment\_elements(

in unsigned long start, in unsigned long how\_many, out AlignmentElementIterator the\_rest) raises(IndexOutOfBounds);

unsigned long num\_rows(); unsigned long num\_columns();

SeqRegion get\_seq\_region( in string key, in Interval the\_interval) raises(ElementNotInAlignment, IntervalOutOfBounds, SeqRegionInvalid);

CompositeSeqRegion get\_seq\_region( in string key, in Interval the\_interval) raises(ElementNotInAlignment, IntervalOutOfBounds, SeqRegionInvalid);

AlignType get\_align\_type\_by\_column(in unsigned long col) raises(IndexOutOfBounds);

};

typedef string AlignType;	
Description:	An <b>AlignType</b> is a <b>string</b> that contains the type of the assumption made for this grouping of regions on sequences. Several kinds of <b>AlignTypes</b> are given below.

typedef sequence <aligntype> AlignTypeList;</aligntype>	
Description:	Used to pass a set of AlignTypes.

I

	ON_PROTEIN = "NON_PROTEIN"; EQUENCE_ERROR = "SEQUENCE_ERROR";
Description:	Common alignment assumptions are provided as simple strings, with constant types as a starting point for a list of assumptions. <b>UNKNOWN</b> indicates that no additional information is provided with the alignment, as would be the case for (e.g., Smith-Waterman alignments). <b>PROTEIN</b> indicates that this column does encode (part of) a protein. This can be either because it contains one or more amino acid residues, or more importantly, because the column consists of triplet(s) of DNA bases that encode amino acid(s). A very common region size is 1 for amino acids, and 3 for nucleotide triplets. However, more complex regions, e.g., a transmembrane protein sequence segment, are entirely possible. <b>SEQUENCE_ERROR</b> indicates that the column contains bases that are considered to be erroneous.
	For example, in aligning a protein to a DNA sequence it possible to distinguish insertions due to evolutionary processes ( <b>PROTEIN</b> ) from insertions due to sequencing error ( <b>SEQUENCE_ERROR</b> ). More involved alignment methods, for example hidden Markov models, could use the <b>AlignType</b> string to provide a sensible decoding of the alignment, and in these cases, the <b>AlignType</b> maybe more informative than the <b>SeqRegion</b> provided by the <b>Alignment</b> .

AlignmentElementList get_alignment_elements( in unsigned long start, in unsigned long how_many, out AlignmentElementIterator the_rest) raises(IndexOutOfBounds);	
Description:	<ul> <li>This method allows the retrieval of AlignmentElements. They correspond to the rows in a traditional textually represented alignment; typically, the AlignmentElements are sequences. Uses the list/iterator hybrid to provide access to the</li> <li>AlignmentElements. A list of no more than how_many elements starting at start is returned as the direct result. The remaining elements, if any, are available through the iterator returned in the out parameter. This is particularly useful for Assemblies, where for a particular region, only a few sequences from thousands are relevant.</li> </ul>
Return value:	Returns an AlignmentElementList containing no more than how_many elements starting at start. The AlignmentElementIterator provides access to any remaining elements to the right of those in AlignmentElementList.
Exceptions:	Raises IndexOutOfBounds if start is less than 1 or more than the number of aligned elements. This upper limit is returned by num_rows().

unsigned long num_rows();	
Description:	The <b>Alignment</b> interface provides access to the <b>AlignmentElements</b> that make up the alignment. The <b>key</b> data member uniquely identifies an <b>AlignmentElement</b> within the <b>Alignment</b> . The total number of <b>AlignmentElements</b> is given by <b>num_rows</b> ().
Return value:	Returns an <b>unsigned long</b> .

unsigned long num_columns();	
Description:	The <b>Alignment</b> interface provides access to the correspondences that make the alignment. The correspondences are numbered 1 to <b>length</b> inclusive, and can be considered the equivalent of alignment columns in a traditional text view of an alignment. The total number of correspondences is given by <b>num_columns</b> ()
Return value:	Returns an unsigned long.

SeqRegion get_seq_region( in string key, in Interval the_interval) raises(ElementNotInAlignment, IntervalOutOfBounds, SeqRegionInvalid);	
Description:	<ul> <li>The input parameter key unambiguously identifies an AlignmentElement within the Alignment. For each correspondence, each AlignmentElement will have a particular SeqRegion, returned by get_seq_region(). A null SeqRegion indicates that there is no region for this correspondence (i.e., a gap). Multiple gaps are represented by multiple SeqRegions. To find the "length" of a gap, it is necessary to check other correspondences in the column. A null SeqRegion contains no length information.</li> <li>The input parameter the_interval represents an interval in the coordinates of the Alignment, not that of the underlying Object. If the interval includes a gap at the start, middle or end, the returned SeqRegion does not show it, because the start and end of it are in the coordinate system of the underlying Object which is unaware of any gaps. Instead, the corresponding segment of the underlying Object is indicated. It is assumed that the numbering of the correspondences is relevant, i.e., that the second correspondence comes after the first, with all the intervals abutting. This allows an Interval of correspondences to be a valid concept.</li> </ul>
Return value:	Returns a SeqRegion.
Exceptions:	Raises ElementNotInAlignment if the AlignmentElement is not associated with this Alignment.         Raises IntervalOutOfBounds if the Interval's start is less than 1 or if its start+length-1 is greater than the total number of correspondences given by num_columns().         Raises SeqRegionInvalid if the_interval is an invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

CompositeSeqRegion get_gaps( in string key, in Interval the_interval) raises(ElementNotInAlignment, IntervalOutOfBounds, SeqRegionInvalid);	
Description:	The input parameter <b>key</b> unambiguously identifies an <b>AlignmentElement</b> within the <b>Alignment</b> . For each correspondence, each <b>AlignmentElement</b> will have gaps returned by <b>get_gaps()</b> . A null <b>CompositeSeqRegion</b> indicates that there are no gaps.
	The input parameter <b>the_interval</b> represents an interval in the coordinates of the <b>Alignment</b> , not that of the underlying <b>Object</b> . It is assumed that the numbering of the correspondences is relevant (i.e., that the second correspondence comes after the first, with all the intervals abutting). This allows an <b>Interval</b> of correspondences to be a valid concept.
Return value:	Returns a <b>CompositeSeqRegion</b> . The <b>start</b> and <b>length</b> of each constituent <b>SeqRegion</b> indicates the location, in the coordinate system of the underlying <b>Object</b> , and number of gaps at that location. Gaps of length 0 are not allowed. A start equal to 0 would be before the first base. A start equal to N is a gap between bases N and N+1. So start equal to the <b>Object's</b> length would be after the last base.
Exceptions:	Raises ElementNotInAlignment if the AlignmentElement is not associated with this Alignment.
	Raises IntervalOutOfBounds if the Interval's start is less than 1 or if its start+length-1 is greater than the total number of correspondences given by num_columns().
	Raises SeqRegionInvalid if the_interval is an invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

AlignType get_align_type_by_column(in unsigned long col) raises(IndexOutOfBounds);	
Description:	<b>get_align_type_by_column</b> () provides a mechanism to retrieve the assumptions used for this correspondence from the <b>Alignment</b> . There is not additional machinery in an <b>Alignment</b> itself to help interpret these <b>AlignTypes</b> . For specific instances of an <b>Alignment</b> constructor, a client that uses the constructor should read the documentation as to how to interpret the <b>AlignType</b> , as it will be part of definition of what the <b>Alignment</b> constructor actually provides. For clients that do not want to interpret the <b>Alignment</b> but would like a sensible representation of it to pass onto other programs or visually to a user, the <b>AlignmentEncoders</b> , <b>CharacterAlignmentEncoder</b> and <b>SingleCharacterAlignmentEncoder</b> will provide an entire server-side solution for the client.
Return value:	Returns an AlignType.
Exceptions:	Raises IndexOutOfBounds if <b>col</b> is less than 1 or greater than the total number of correspondences given by <b>num_columns</b> ().

### AlignmentList

I

typedef sequence <alignment> AlignmentList;</alignment>	
Description:	Used to pass a set of Alignments.

# 2.1.16 Alignment Examples

The precise interpretation of this specification for alignments is illustrated with a number of examples. Firstly a standard protein multiple alignment is provided, and secondly a more complicated, protein to EST sequence tag alignment is presented.

### **Protein Multiple Alignment**

This alignment is a fragment of an alignment from the Pfam database. A text representation of this alignment is given below.

CAJ1_YEAST/6-24	EYYDILGIKPEATPTEIKK
YIS4_YEAST/6-24	EYYDLLGVSTTASSIEIKK
YNW7_YEAST/4-22	CYYELLGVETHASDLELKK
YGM8_YEAST/79-104	NLYDVLELPTPLDVHTIYDDLPQIKR

The Alignment object which represented this would return four AlignmentElement objects from the get\_alignment\_elements() method. The first object would have the AminoAcidSequence Object that presented the sequence CAJ1\_YEAST in the

element attribute and the **SeqRegion** would have the **start** attribute of 6 and a **length** attribute of 19. Calling the **get\_seq\_region**() method with this **AlignmentElement** and an **Interval** of **start** 1, **length** 1 would provide a **SeqRegion** with **start** 6, **length** 1, being the sixth residue in CAJ1\_YEAST, a Glutamate 'E'. The following table shows the results of this call to **get\_seq\_region**() and several other similar calls, each with different input **Intervals**. All calls are for the sequence CAJ1\_YEAST.

string	qRegion	out Interval output Seq		put Interval output SeqRegion		input I
	length	start	length	start		
a Glutamate 'E'	1	6	1	1		
a Tyrosine 'Y'	1	7	1	2		
the peptide "YYD"	3	7	3	2		
a gap '-'	null		1	11		
a gap '-'	null		1	12		
the peptide "EATP"	4	16	10	12		

Table 2-5 Call Results

The **get\_align\_type\_by\_column()** method would return either **UNKNOWN** or **PROTEIN** depending on the implementor. Potentially, if the alignment had been made with a more involved method, for example, a hidden Markov model with a notion of structural state, the structural state that was used in each column could be returned.

Of course, for clients whose main purpose is display, the laborious business of querying each position for the region and then looking into the sequence object for the residue at that position is a convoluted route for retrieving the information. If the implementor provided a **CharacterAlignmentEncoder** for this **Alignment**, then a text representation of the **Alignment** could be quickly retrieved and displayed, potentially using the large-scale transport methods provided in

**SingleCharacterAlignmentEncoder** as this alignment has a single character per correspondence. Once displayed, a client could quickly interpret a query on a particular character in the alignment, as it would simply have to call **get\_seq\_region()** with the column position to retrieve the position in the sequence.

#### Protein vs. EST alignment

This example is of a drosophila protein compared to an EST sequence with a frame-shift error occurring, as one would find in GCG's FrameSearch, FASTX, and Wise2. A fragment of the alignments is shown in the following table.

| |

column	20	21	22	23
EST	111-113 (codon)	114-116 (codon)	117	118-120 (codon)
protein	55	56		57
AlignType	PROTEIN	PROTEIN	SEQUENCE_ERROR	PROTEIN

Table 2-6 Protein vs. EST Alignment

The Alignment would have two **AlignmentElements**, one with the EST and one with the protein. Querying the Alignment with the **get\_seq\_region()** method would reveal the sequence regions listed above for each of the sequences. More importantly, the **get\_align\_type\_by\_column()** method for Column 22 would return a type **SEQUENCE\_ERROR**, whereas for the other columns it would return a type **PROTEIN**. This way a program can confidently interpret the alignment. To indicate how important this information is, imagine if in Column 22 three bases were aligned. It would be ambiguous as to whether this indicated a protein insertion of a codon or a sequence error. The **AlignType** here provides this additional information.

The ability to associate a **CharacterAlignmentEncoder** with a more complex **Alignment** as this example is provides a way for clients to retrieve both the **Alignment** and a desired interpretation of the **Alignment** from the server, which facilitates writing alignment clients separately from actual alignment constructors. The **AlignmentEncoder**s provide a route for at least a character-based representation of the **Alignment** to be provided by the server, however complex the alignment method is. In this case, one might have one **AlignmentEncoder**, which provided the amino acids from the protein as three letter codes lined up with three bases from the EST. A different encoder might use one letter amino acid codes throughout, and not show the DNA sequence at all, choosing to encode the sequencing error with a special character.

### 2.1.17 Assembly

**Assembly** extends **Alignment**. **Assembly** contains no additional functionality. The technical domain is evolving rapidly and it's not clear what additional functionality will be necessary. However, the submitters believe it is important to establish the relationship between **Assembly** and **Alignment**.

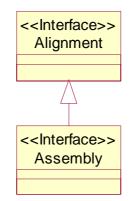


Figure 2-16 The Assembly Interface

interface Assembly : Alignment
{
};

# 2.1.18 SearchHit

The **SearchHit** valuetype provides a generic mechanism to return the results of some type of query against a collection of **BioSequence** objects. The **SearchHit** provides information about a particular sequence that was found and associated information for this hit relevant to this particular search, for an example, a score.

The **SearchHit** valuetype is used as a base class for the **SimilaritySearchHit**, which provides a specialization of the **SearchHit** for similarity searches

<<valuetype>> SearchHit

id : Identifier hit\_info : CosPropertyService::Properties

Figure 2-17 The SearchHit valuetype

### SearchHit

```
valuetype SearchHit
{
    public Identifier id;
    public CosPropertyService::Properties hit_info;
};
```

public Identifier id;	
Description:	The <b>Identifier</b> string identifies a sequence. It can be used with a <b>BioSequenceIdentifierResolver</b> to access the actual sequence.
Return value:	Returns an <b>Identifier</b> string. <b>id</b> shall not be empty.

public CosPropertyService::Properties hit_info;	
Description:	The <b>hit_info</b> provides additional information that is not contained in the <b>BioSequence</b> but is relevant from the perspective of the search. Common information would be the score in a similarity comparison, the statistical probability of the hit or the relevance of the hit in a text search. Content and type of information returned will vary with analysis type.
Return value:	Returns a CosPropertyService::Properties.

The following BLAST example illustrates the type of information that would be placed in **hit\_info**. The example is taken from NCBI's BLAST help page. The associated alignment information is discussed below in the description of **SimilaritySearchHit**.

```
Smallest

Sum

High Probability

Sequences producing High-scoring Segment Pairs: Score P(N) N

sp|P05120|PAI2_HUMAN PLASMINOGEN ACTIVATOR INHIBITOR-2, P... 176 1.8e-65 4

[information deleted - ed.]

>sp|P05120|PAI2_HUMAN PLASMINOGEN ACTIVATOR INHIBITOR-2, PLACENTAL (PAI-2)

(MONOCYTE ARG- SERPIN).

Length = 415

Score = 176 (80.2 bits), Expect = 1.8e-65, Sum P(4) = 1.8e-65

Identities = 38/89 (42%), Positives = 50/89 (56%)
```

### SearchHitList

typedef sequence <searchhit> SearchHitList;</searchhit>	
Description:	Used to pass a set of <b>SearchHits</b> .

### SearchHitIterator

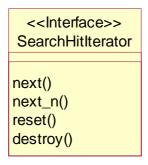


Figure 2-18 The SearchHitIterator Interface

#### interface SearchHitlterator

{		
•	boolean	next(out SearchHit hit)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out SearchHitList hit_list)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		

boolean next(out SearchHit hit) raises(IteratorInvalid);		
Description:	The <b>next()</b> operation gets the next <b>SeachHit</b> in its out parameter <b>hit</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>hit</b> parameter to null.	
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

boolean next_n(in unsigned long how_many, out SearchHitList hit_list) raises(IteratorInvalid);	
Description:	next_n() returns SearchHits in the SearchHitList out parameter hit_list, containing at most the number specified in the first parameter (how_many) and returns a boolean value directly. When it is at the end of the set it returns FALSE and the hit_list parameter will have length zero. In all cases the length of hit_list will be the minimum of how_many and the number of elements remaining.
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

void reset();	
Description:	reset() sets the iterator to the start of the set.
Exceptions:	Raises CORBA::NO_IMPLEMENT with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).

void destroy();	
Description:	destroy() frees the iterator object.

# 2.1.19 SimilaritySearchHit

The **SimilaritySearchHit** valuetype provides a specialization of the **SearchHit** valuetype for searches of **BioSequence** collections that are on the basis of similarity, such as BLAST, Fasta, or Smith-Waterman searches.

The member **alignment\_list** is added to the **SearchHit** valuetype. This **AlignmentList** contains the details of a similarity search hit in the form of an **Alignment**. This list will frequently be of length one, but can be used to group all "local" hits pertaining to a single found sequence into one **SimilaritySearchHit**. That is, one **SimilaritySearchHit** may contain one "local match" or several "local matches" on one sequence. What is most appropriate depends on the analysis that was run to obtain the hits, and/or on the objective of a service; an implementation must document these semantics.

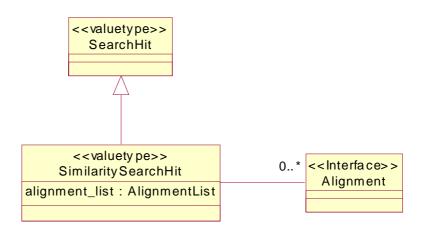


Figure 2-19 The SimilaritySearchHit valuetype

# valuetype SimilaritySearchHit : SearchHit { public AlignmentList alignment\_list;

};

public AlignmentList alignment_list;	
Description:	This attribute provides a list of <b>Alignments</b> that are associated with this hit. Not all hits may have alignments. In the <b>Alignments</b> , the sequence or object that was used as a query is the first <b>AlignmentElement</b> and the other objects (in most cases, just one) follow.
	If the <b>alignment_list</b> contains more than one <b>Alignment</b> , each <b>Alignment</b> shall involve the same two objects, i.e., only two <b>Identifiers</b> are used within one <b>SimilaritySearchHit</b> , one for the initial <b>query_sequence</b> (see <b>SearchHit</b> ) and one for the current target sequence.
	Since each <b>Alignment</b> in a <b>SimilaritySearchHit</b> is a pairwise alignment, the result of the <b>Alignment's num_rows</b> () method shall be 2.
Return value:	Returns a list of <b>Alignments</b> .

The following BLAST example illustrates the alignment information that may be associated with a **SimilaritySearchHit**. The example is taken from NCBI's BLAST help page.

```
>sp|P05120|PAI2_HUMAN PLASMINOGEN ACTIVATOR INHIBITOR-2, PLACENTAL (PAI-2)
           (MONOCYTE ARG- SERPIN).
           Length = 415
Score = 176 (80.2 bits), Expect = 1.8e-65, Sum P(4) = 1.8e-65
Identities = 38/89 (42%), Positives = 50/89 (56%)
          1 QIKDLLVSSSTDLDTTLVLVNAIYFKGMWKTAFNAEDTREMPFHVTKQESKPVQMMCMNN 60
Query:
                   +I +LL S D DT +VLVNA+YFKG WKT F + PF V
                                                                 + PVOMM +
Sbjct:
        180 KIPNLLPEGSVDGDTRMVLVNAVYFKGKWKTPFEKKLNGLYPFRVNSAQRTPVQMMYLRE 239
         61 SFNVATLPAEKMKILELPFASGDLSMLVL 89
Query:
                     N+ + K +ILELP+A L+L
Sbjct:
        240 KLNIGYIEDLKAQILELPYAGDVSMFLLL 268
```

#### SimilaritySearchHitList

typedef sequence <similaritysearchhit> SimilaritySearchHitList;</similaritysearchhit>	
Description:	Used to pass a set of SimilaritySearchHits.

This **AlignmentList** contains the details of a similarity search hit in the form of an **Alignment**. This list will frequently be of length one, but can be used to group all "local" hits pertaining to a single found sequence into one **SimilaritySearchHit**. That is, one **SimilaritySearchHit** may contain one "local match" or several "local matches" on one sequence. What is most appropriate depends on the analysis that was run to obtain the hits, and/or on the objective of a service; an implementation must document these semantics.

## 2.1.20 BioSequenceIdentifierResolver

The **BioSequenceIdentifierResolver** provides a mechanism to retrieve the actual **BioSequence** object from a collection search, using the **Identifier** string.

Implementors may want to consider multiply inheriting from **BioSequenceIdentifierResolver** interface with the optional **BioSequence** factories to provide sequence creation for an **Identifier**.

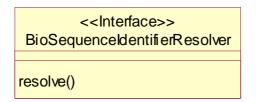


Figure 2-20 The BioSequenceIdentifierResolver interface

```
interface BioSequenceIdentifierResolver
{
BioSequence resolve(in Identifier id)
raises (IdentifierNotFound, IdentifierNotResolvable,
IdentifierNotUnique);
```

};

BioSequence resolve(in Identifier id) raises (IdentifierNotFound, IdentifierNotResolvable, IdentifierNotUnique);	
Description:	The <b>resolve()</b> method provides the <b>BioSequence</b> for the particular <b>Identifier</b> .
Return value:	Returns a <b>BioSequence</b> .
Exceptions:	Raises IdentifierNotFound if the database and the identifier within the database can be resolved but the Identifier is not present.
	Raises IdentifierNotResolvable if the database and the identifier within the database cannot be resolved such that the <b>Identifier</b> cannot even be searched for.
	Raises IdentifierNotUnique if the Identifier specification is ambiguous and returns more than one object.

## 2.1.21 SearchResult

The **SearchResult** interface provides the complete results of a single search against a collection of **BioSequences**, including the individual hits and their associated scores and information about the search as whole. This interface is designed to represent results from both similarity queries on a database (such as BLAST, Fasta or Smith-Waterman) and text based searches on a database of **BioSequences**.

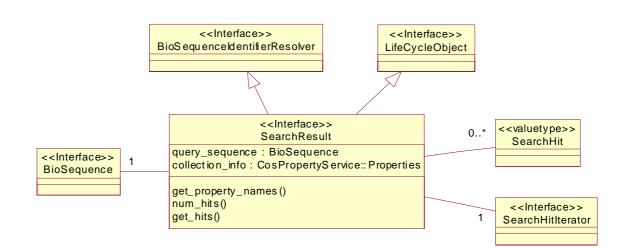


Figure 2-21 The SearchResult Interface

#### SearchResult

The SearchResult interface inherits from the BioSequenceIdentifierResolver to allow the retrieval of the actual **BioSequences** from the collection. It also inherits from CosLifeCycle::LifeCycleObject to allow management of its resources.

```
interface SearchResult :
    BioSequenceIdentifierResolver.
    CosLifeCycle::LifeCycleObject
    readonly attribute BioSequence query_sequence;
    readonly attribute CosPropertyService::Properties collection_info;
    StringList get_property_names();
    unsigned long num_hits();
    SearchHitList get_hits(
```

in unsigned long start, in unsigned long how\_many, out SearchHitlterator the\_rest) raises (IndexOutOfBounds);

};

{

readonly attribute BioSequence query_sequence;	
Description:	This attribute provides the query sequence that was used in this <b>SearchResult</b> . It may be null in the case of non similarity based searches.
Return value:	Returns a <b>BioSequence</b> .

readonly attribute CosPropertyService::Properties collection_info;	
Description:	The <b>collection_info</b> provides additional information that is not contained in the <b>SearchHits</b> but is relevant from the perspective of the search. Common information would be the database Identifier, the number of sequences in the database, and some statistical information about the search.
Return value:	Returns a CosPropertyService::Properties.

The following BLAST example illustrates the type of information that could be placed in **collection\_info**. The example is taken from NCBI's BLAST help page.

```
BLASTP 1.4.6MP [13-Jun-94] [Build 13:58:36 Sep 22 1994]
Reference: Altschul, Stephen F., Warren Gish, Webb Miller, Eugene W. Myers,
and David J. Lipman (1990). Basic local alignment search tool. J. Mol. Biol.
215:403-10.
Query = pir | A01243 | DXCH 232 Gene X protein - Chicken (fragment)
           (232 letters)
Database: SWISS-PROT Release 29.0
                    38,303 sequences; 13,464,008 total letters.
Searching.....done
    Observed Numbers of Database Sequences Satisfying
    Various EXPECTation Thresholds (E parameter values)
     Histogram units:
                      = 31 Sequences : less than 31 sequences
EXPECTation Threshold
(E parameter)
  V Observed Counts-->
 10000
                  4863
                       6310
                  3002
                         812 |========================
 3980
                  2220
                         303 ========
 2510
                 1408
 1580
                 1105
                         1000
                  712
                         179 |=====
  631
                  533
                         161 |=====
  398
                  372
                          80 ==
  251
                  292
                          73 |==
                  219
                          50 =
  158
                          32 |=
  100
                  169
 63.1
                  137
                          18 |:
 39.8
                           9 |:
                  119
                           6 |:
 25.1
                  110
                          9 |:
 15.8
                  104
```

10.0 95 4 |: 3 |: 6.31 91 1 : 3.98 88 2.51 87 3 |: 1.58 84 0 | 1.00 84 2 |: [SearchHit information deleted - ed.] WARNING: HSPs involving 86 database sequences were not reported due to the limiting value of parameter B = 9. Parameters: V=15 B=9 H=1-ctxfactor=1.00 E = 10----- As Used -----Query ---- Computed ----Lambda K H Н MatID Matrix name Frame Lambda K 0.316 0.132 0.370 same +0 0 BLOSUM62 same same Query Frame MatID Length Eff.Length E S W T X E2 S2 10. 57 3 11 22 +0 0 232 232 0.22 33 Statistics: HSPs HSPs Query Expected Observed High Score MatID High Score Frame Reportable Reported 62 (28.2 bits) 1191 (542.5 bits) 330 +0 0 2.4 Query Neighborhd Word Excluded Failed Successful Overlaps Hits Frame MatID Words Hits Extensions Extensions Excluded 4988 5661199 1146395 4504598 10187 +00 13 Database: SWISS-PROT Release 29.0 Release date: June 1994 Posted date: 1:29 PM EDT Jul 28, 1994 # of letters in database: 13,464,008 # of sequences in database: 38,303 # of database sequences satisfying E: 95 No. of states in DFA: 561 (55 KB) Total size of DFA: 110 KB (128 KB) Time to generate neighborhood: 0.03u 0.01s 0.04t Real: 00:00:00 No. of processors used: 8 Time to search database: 32.27u 0.78s 33.05t Real: 00:00:04 Total cpu time: 32.33u 0.91s 33.24t Real: 00:00:05 WARNINGS ISSUED: 2

StringList get_property_names();	
Description:	The names of the <b>hit_info</b> properties in <b>SearchHit</b> are available here so that clients have access to them before processing the list of <b>SearchHits</b> .
Return value:	Returns a StringList.

unsigned long num_hits();	
Description:	Provides the number of hits in this <b>SearchResult</b> .
Return value:	Returns an <b>unsigned long</b> .

SearchHitList get_hits( in unsigned long start, in unsigned long how_many, out SearchHitIterator the_rest) raises (IndexOutOfBounds);	
Description:	Uses the list/iterator hybrid to provide access to the actual <b>SearchHits</b> , which could be <b>SimilaritySearchHits</b> . A list of no more than <b>how_many</b> hits starting at <b>start</b> is returned as the direct result. The remaining elements, if any, are available through the iterator returned in the <b>out</b> parameter.
Return value:	Returns a SearchHitList.
Exceptions:	Raises IndexOutOfBounds if the index is less than 1 or greater than the number of hits in the <b>SearchResult</b> . This upper limit is returned by <b>num_hits()</b> .

The method **get\_hits**() returns a list of **SearchHits**. If this concerns **SimilaritySearchHits**, then these elements will in turn contain a list of **Alignments**. The latter can be used to group all "local" hits pertaining to a single found sequence into one **SimilaritySearchHit**. That is, one **SimilaritySearchHit** may contain one "local match" or several "local matche"' on one sequence. What is most appropriate depends on the analysis that was run to obtain the hits, and/or on the objective of a service. An implementation must document these semantics.

## 2.1.22 AnnotationFactory (Optional)

AnnotationFactory provides a means of creating new Annotation and SeqAnnotation objects. This permits a clean separation of factory issues from the Annotation objects themselves. Annotations are created via the factory method **create\_annotation()**, which accepts all of the components. Similarly, **SeqAnnotations** are created via the factory method **create\_seq\_annotation()**, which accepts all of the components.

AnnotationFactory is an optional compliance point of this specification.

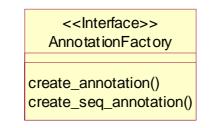


Figure 2-22 The AnnotationFactory Interface

```
interface AnnotationFactory
{
    Annotation create_annotation(
        in string name,
        in any value,
        in Basis the_basis,
        in CosPropertyService::Properties qualifiers);
    SeqAnnotation create_seq_annotation(
        in string name,
        in any value,
        in Basis the_basis,
        in CosPropertyService::Properties qualifiers,
        in CosPropertyService::Properties qualifiers,
        in SeqRegion seq_region)
        raises(SeqRegionInvalid);
```

};

Annotation create_annotation( in string name, in any value, in Basis the_basis, in CosPropertyService::Properties qualifiers);	
Description:	The <b>create_annotation()</b> operation creates an <b>Annotation</b> and populates it with the supplied attributes. No error checking is performed.
Return value:	Returns an <b>Annotation</b> with the appropriate content.

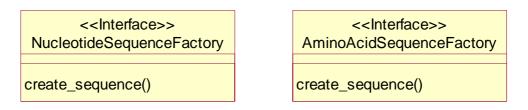
SeqAnnotation create_seq_annotation( in string name, in any value, in Basis the_basis, in CosPropertyService::Properties qualifiers, in SeqRegion seq_region) raises(SeqRegionInvalid);	
Description:	The <b>create_seq_annotation()</b> operation creates a <b>SeqAnnotation</b> and populates it with the supplied attributes. No error checking is performed.
Return value:	Returns a <b>SeqAnnotation</b> with the appropriate content.
Exceptions:	Raises SeqRegionInvalid if the seq_region parameter is deemed invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

## 2.1.23 BioSequence factories (Optional)

Sequence factories permit a clean separation of object vending from **BioSequence** data model issues. **BioSequence** factories are an optional compliance point of this submission.

**BioSequence** factories provide a means of creating new **NucleotideSequence** and **AminoAcidSequence** objects. Sequences are created via the factory method **create\_sequence()**, which accepts all of the components.

Implementors may want to consider mixing in the **BioSequenceIdentifierResolver** interface to provide sequence creation for an **Identifier**.





## SeqAnnotationOutOfBounds

exception SeqAnnotationOutOfBounds { SeqAnnotation invalid; Interval valid; };	
Description:	The SeqAnnotationOutOfBounds exception is raised if a SeqAnnotation's SeqRegion has a start less than 1 or if its start+length-1 is greater than the length of the BioSequence. The exception is also raised if a nested sub- region of a CompositeSeqRegion is invalid. If a BioSequence represents circular DNA, then this exception should be raised if the Interval's start is less than 1 or greater than the length of the BioSequence, or if its length is greater than that of the BioSequence.
Return value:	Returns the invalid SeqAnnotation and the valid Interval. The valid Interval has start equal to 1 and length equal to the length of the BioSequence, the largest allowed Interval.

#### *NucleotideSequenceFactory*

NucleotideSequenceFactory provides a means of creating new NucleotideSequences. NucleotideSequenceFactory is an optional compliance point of this specification.

interface NucleotideSequenceFactory

{

NucleotideSequence create\_sequence(

- in string name,
- in Identifier id,
- in string description,
- in string residues,
- in Basis the\_basis,
- in boolean circular,
- in AnnotationList annotations)

raises (InvalidResidue, SeqAnnotationOutOfBounds, SeqRegionInvalid);

2

};

I

NucleotideSequence create_sequence( in string name, in Identifier id, in string description, in string residues, in Basis the_basis, in boolean circular, in AnnotationList annotations) raises (InvalidResidue, SeqAnnotationOutOfBounds, SeqRegionInvalid);	
Description:	The <b>create_sequence()</b> operation creates a <b>NucleotideSequence</b> and populates it with the supplied attributes. No error checking is performed except on the residues, which must be valid IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes. The residues need not be upper-case. <b>BioSequenceIdentifierResolver</b> can be mixed in to provide lookup based on sequence ID.
Return value:	Returns a <b>NucleotideSequence</b> with the appropriate content.
Exceptions:	Raises InvalidResidue if the string of residues is inconsistent with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes. Note that residue is interpreted to mean base here (see Glossary). Raises SeqAnnotationOutOfBounds if annotations contains a SeqAnnotation whose seq_region is out of bounds for this BioSequence. Raises SeqRegionInvalid if the annotations parameter contains SeqAnnotation having a seq_region attribute that is deemed invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g.,
	one that has a wrong <b>SeqRegionOperator</b> or contains overlaps or circularities).

## AminoAcidSequenceFactory

AminoAcidSequenceFactory provides a means of creating new AminoAcidSequences. AminoAcidSequenceFactory is an optional compliance point of this specification.

interface AminoAcidSequenceFactory
{

AminoAcidSequence create\_sequence(

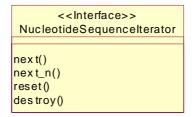
- 2
- in string name, in Identifier id, in string description, in string residues, in Basis the\_basis, in AnnotationList annotations) raises (InvalidResidue, SeqAnnotationOutOfBounds, SeqRegionInvalid);
- };

AminoAcidSequence create_sequence( in string name, in Identifier id, in string description, in string residues, in Basis the_basis, in AnnotationList annotations) raises (InvalidResidue, SeqAnnotationOutOfBounds, SeqRegionInvalid);	
Description:	The <b>create_sequence()</b> operation creates an <b>AminoAcidSequence</b> and populates it with the supplied attributes. No error checking is performed except on the residues, which must be valid IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes. The residues need not be upper-case. <b>BioSequenceIdentifierResolver</b> can be mixed in to provide lookup based on sequence ID.
Return value:	Returns a <b>AminoAcidSequence</b> with the appropriate content.
Exceptions:	<ul> <li>Raises InvalidResidue if the string of residues is inconsistent with the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) single letter codes.</li> <li>Raises SeqAnnotationOutOfBounds if annotations contains a SeqAnnotation whose seq_region is out of bounds for this BioSequence.</li> <li>Raises SeqRegionInvalid if the annotations parameter contains SeqAnnotation having a seq_region attribute that is deemed invalid. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).</li> </ul>

## 2.1.24 BioSequence iterators (Optional)

Iterator specifications are defined for iterating over a set of **BioSequence**, **NucleotideSequence**, or **AminoAcidSequence** objects. **NucleicAcidIterator** and **AminoAcidIterator** are specialized versions of **BioSequenceIterator** having the same operations but with signatures specialized for the corresponding **BioSequence** sub-types. **BioSequenceIterator** and **BioSequenceList** may contain both **NucleotideSequences** and **AminoAcidSequences**. Homogeneity in the sequence types of iterators and lists can be achieved using the specialized versions.

< <interface>&gt; BioSequenceIterator</interface>
next() next_n() reset() destroy()



Ami	< <interface>&gt; noAcidSequenceIterator</interface>
next( next_ reset destr	()

Figure 2-24 The BioSequence Iterators

#### **BioSequenceIterator**

**BioSequencelterator** provides a strongly typed iterator for **BioSequences**.

interface BioSequenceIterator

{		
•	boolean	next(out BioSequence seq)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out BioSequenceList seqs)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
٦.		

};

boolean next(out BioSequence seq) raises(IteratorInvalid);	
Description:	The <b>next()</b> operation gets the next <b>BioSequence</b> in its out parameter <b>seq</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>seq</b> parameter to null.
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

boolean next_n(in unsigned long how_many, out BioSequenceList seqs) raises(IteratorInvalid);	
Description:	<ul> <li>next_n() returns BioSequences in the BioSequenceList out parameter seqs, containing at most the number specified in the first parameter (how_many) and returns a boolean value directly. When it is at the end of the sequence set it returns FALSE and the seqs parameter will have length zero. In all cases the length of seqs will be the minimum of how_many and the number of sequences remaining.</li> </ul>
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).

void reset();	
Description:	reset() sets the iterator to the start of the set.
Exceptions:	Raises <b>CORBA</b> ::NO_IMPLEMENT with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).

void destroy();	
Description:	destroy() frees the iterator object.

## NucleotideSequenceIterator

**NucleotideSequencelterator** provides a strongly typed iterator for **NucleotideSequences**.

interface NucleotideSequenceIterator

{		
•	boolean	next(out NucleotideSequence seq)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out NucleotideSequenceList seqs)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		

boolean next(out NucleotideSequence seq) raises(IteratorInvalid);		
Description:	The <b>next()</b> operation gets the next <b>NucleotideSequence</b> in its out parameter <b>seq</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>seq</b> parameter to null.	
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

boolean next_n(in unsigned long how_many, out NucleotideSequenceList seqs) raises(IteratorInvalid);		
Description:	<pre>next_n() returns NucleotideSequences in the NucleotideSequenceList out parameter seqs, containing at most the number specified in the first parameter (how_many) and returns a boolean value directly. When it is at the end of the sequence set it returns FALSE and the seqs parameter will have length zero. In all cases the length of seqs will be the minimum of how_many and the number of sequences remaining.</pre>	
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>lteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

void reset();		
Description:	reset() sets the iterator to the start of the set.	
Exceptions:	Raises <b>CORBA</b> ::NO_IMPLEMENT with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).	

void destroy();	
Description:	destroy() frees the iterator object.

\_\_\_\_\_

## AminoAcidSequenceIterator

AminoAcidSequencelterator provides a strongly typed iterator for AminoAcidSequences.

## interface AminoAcidSequenceIterator

{		
•	boolean	next(out AminoAcidSequence seq)
		raises(IteratorInvalid);
	boolean	next_n(in unsigned long how_many,
		out AminoAcidSequenceList seqs)
		raises(IteratorInvalid);
	void	reset();
	void	destroy();
};		
};		

boolean next(out AminoAcidSequence seq) raises(IteratorInvalid);		
Description:	The <b>next()</b> operation gets the next <b>AminoAcidSequence</b> in its out parameter <b>seq</b> and returns a boolean value. If the iterator is at the end of the set, it returns FALSE and sets the output <b>seq</b> parameter to null.	
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

boolean next_n(in unsigned long how_many, out AminoAcidSequenceList seqs) raises(IteratorInvalid);		
Description:       next_n() returns AminoAcidSequences in the         AminoAcidSequenceList out parameter seqs, containing         the number specified in the first parameter (how_many) and         boolean value directly. When it is at the end of the sequence         returns FALSE and the seqs parameter will have length zero         cases the length of seqs will be the minimum of how_many         number of sequences remaining.		
Return value:	Returns FALSE if the iterator is at the end of the set and TRUE otherwise.	
Exceptions:	Raises <b>IteratorInvalid</b> if the iterator is no longer valid (e.g., the underlying collection has changed).	

void reset();		
Description: <b>reset()</b> sets the iterator to the start of the set.		
Exceptions:	Raises <b>CORBA</b> :: <b>NO_IMPLEMENT</b> with standard minor code 5 if the iterator cannot be reset (e.g., the iterator provides access to streaming data).	

void destroy();	
Description:	destroy() frees the iterator object.

# 2.1.25 GeneticCodeFactory (Optional)

**GeneticCodeFactory** provides a means of creating new **GeneticCodes**. **GeneticCodeFactory** is an optional compliance point of this specification.

## InvalidGeneticCodeName

exception InvalidGeneticCodeName { string invalid_name; };		
Description:	The InvalidGeneticCodeName exception is raised when an invalid GeneticCodeName is passed to GeneticCodeFactory's create_genetic_code().	
Return value:	Returns a <b>string</b> containing the invalid name.	

### Genetic Code Factory

The GeneticCodeFactory interface defines a set of const GeneticCodeName strings that list the set of currently known genetic codes. The genetic\_code\_names attribute provides access to the supported GeneticCodeNames. create\_genetic\_code() creates the appropriate GeneticCode. Codings for the GeneticCodeNames listed below can be found in Appendix B.

GeneticCodeFactory	
STANDARD : GeneticCodeName = "standard"	
BACTERIAL : GeneticCodeName = "bacterial"	
YEAST_MITOCHONDRIAL : GeneticCodeName = "yeast mitochondrial"	
VERTEBRATE_MITOCHONDRIAL : GeneticCodeType = "vertebrate mitochondrial"	
MOLD_MITOCHONDRIAL : GeneticCodeName = "mold mitochondrial"	
IN VERTEBRATE_MITOCHONDRIAL : GeneticCodeName = "invertebrate mitochond	drial"
ECHINODERM_MITOCHONDRIAL: GeneticCodeName = "echinoderm mitochondr	ia I"
ASCIDIAN_MITOCHONDRIAL : GeneticCodeName = "ascidian mitochondrial"	
FLATW ORM _MITOCHONDRIAL : GeneticCodeName = "flatworm mitochondrial"	
CILIATE_NUCLEAR : GeneticCodeName = "ciliate nuclear"	
EUPLOTID_NUCLEAR : GeneticCodeName = "euplotid nuclear"	
ALT_YEAST_NUCLEAR : GeneticCodeName = "alternative yeast nuclear"	
BLEPHARISMA_MACRONUCLEAR : GeneticCodeName = "blepharisma macronuc	lear"
genetic_code_names:GeneticCodeNameList	

create\_genetic\_code()

Figure 2-25 The GeneticCodeFactory Interface

interface GeneticCodeFactory

{			
-	const GeneticCodeName	STANDARD	= "standard";
	const GeneticCodeName	BACTERIAL	= "bacterial";
	const GeneticCodeName	YEAST_MITOCHONDRIAL	= "yeast mitochondrial";
	const GeneticCodeName	VERTEBRATE_MITOCHONDRIAL	= "vertebrate mitochondrial";
	const GeneticCodeName	MOLD_MITOCHONDRIAL	= "mold mitochondrial";
	const GeneticCodeName	INVERTEBRATE_MITOCHONDRIAL	= "invertebrate mitochondrial";
	const GeneticCodeName	ECHINODERM_MITOCHONDRIAL	= "echinoderm mitochondrial";
	const GeneticCodeName	ASCIDIAN_MITOCHONDRIAL	= "ascidian mitochondrial";
	const GeneticCodeName	FLATWORM_MITOCHONDRIAL	= "flatworm mitochondrial";
	const GeneticCodeName	CILIATE_NUCLEAR	= "ciliate nuclear";
	const GeneticCodeName	EUPLOTID_NUCLEAR	= "euplotid nuclear";
	const GeneticCodeName	ALT_YEAST_NUCLEAR	= "alternative yeast nuclear";
	const GeneticCodeName	BLEPHARISMA_MACRONUCLEAR	= "blepharisma macronuclear";

readonly attribute GeneticCodeNameList genetic\_code\_names; GeneticCode create\_genetic\_code(in GeneticCodeName name) raises(InvalidGeneticCodeName);

};

const GeneticCoo const GeneticCoo	deName       STANDARD         deName       BACTERIAL         deName       YEAST_MITOCHONDRIAL         deName       VERTEBRATE_MITOCHONDRIAL         deName       MOLD_MITOCHONDRIAL         deName       MOLD_MITOCHONDRIAL         deName       ECHINODERM_MITOCHONDRIAL         deName       ECHINODERM_MITOCHONDRIAL         deName       FLATWORM_MITOCHONDRIAL         deName       FLATWORM_MITOCHONDRIAL         deName       EUPLOTID_NUCLEAR         deName       ALT_YEAST_NUCLEAR         deName       BLEPHARISMA_MACRONUCLEAR	<ul> <li>"standard";</li> <li>"bacterial";</li> <li>"yeast mitochondrial";</li> <li>"vertebrate mitochondrial";</li> <li>"mold mitochondrial";</li> <li>"invertebrate mitochondrial";</li> <li>"echinoderm mitochondrial";</li> <li>"ascidian mitochondrial";</li> <li>"flatworm mitochondrial";</li> <li>"ciliate nuclear";</li> <li>"euplotid nuclear";</li> <li>"alternative yeast nuclear";</li> <li>"blepharisma macronuclear";</li> </ul>
Description:	The <b>GeneticCodeFactory</b> interface defines a set of <b>const GeneticCodeName</b> strings that list the set of currently known genetic codes. The <b>GeneticCodeName</b> defines the particular <b>Coding</b> that is used to convert <b>Codons</b> into <b>Residues</b> so one need only specify the <b>GeneticCodeName</b> when creating a <b>GeneticCode</b> object from one of the known types. <b>Codings</b> for the <b>GeneticCodeNames</b> listed above can be found in Appendix B.	

readonly attribute GeneticCodeNameList genetic_code_names;	
Description:	The <b>genetic_code_names</b> attribute provides access to the supported <b>GeneticCodeNames</b> .
Return value:	Returns a GeneticCodeNameList.

GeneticCode create_genetic_code(in GeneticCodeName name) raises(InvalidGeneticCodeName);	
Description:	<b>create_genetic_code()</b> creates the appropriate <b>GeneticCode</b> corresponding to the <b>GeneticCodeName</b> . <b>Codings</b> for the <b>GeneticCodeNames</b> listed above can be found in Appendix B.
Return value:	Returns a GeneticCode.
Exceptions:	Raises InvalidGeneticCodeName if the GeneticCodeName is not supported (i.e., returned by the genetic_code_names attribute).

## 2.1.26 CharacterAlignmentEncoder (Optional)

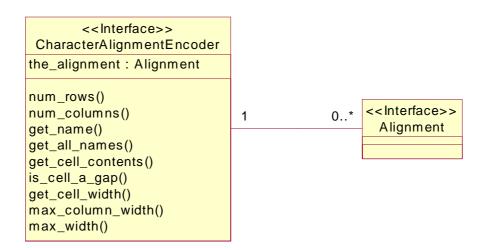
The **CharacterAlignmentEncoder** and its specialization **SingleCharacterAlignmentEncoder** are optional parts of the specification that facilitate the representation of the **Alignment** for thin clients. It is important that these

interfaces have a proposed standard, as it will allow clients that do not want to investigate **Alignments** directly to get useful information for passing on to a user or to another, text format based application.

A **CharacterAlignmentEncoder**'s role is to produce string text similar to that in Table 2-4 on page 2-43, with columns of text indicating the correspondences and the row indicating each sequence. The exact format isn't specified or standardized. The factory that makes the encoder will govern the precise nature of the encoding, such as what pad character is used. The **CharacterAlignmentEncoder** might have more than one character per column, allowing the transmission of three-letter amino acid code or more than one base of DNA sequence in a single column. To allow the client to format the resulting data, **max\_column\_width()** returns the maximum length of characters in a column. Rows and columns are numbered starting at 1.

The **Alignment** and the **CharacterAlignmentEncoder** interfaces work well for both view-based clients and programmatic clients. The interfaces provide viewing clients with an easy, low cost route of gathering the alignment data and displaying it to the user. The coordinate system of the string encoded alignment maps to the underlying alignment, allowing the client to retrieve specific regions of the alignment of interest. Since the **Interval** valuetype can be used to retrieve only portions of the **BioSequences**, these very complex objects can remain on the server, with the clients displaying only portions of interest to the user. For programmatic clients wanting to use the alignment as the basis of further analysis, the **Alignment** interface provides a mapping system of moving from one sequence to another sequence via the alignment.

**CharacterAlignmentEncoder** is an optional compliance point of this specification.





#### interface CharacterAlignmentEncoder

{

I

readonly attribute Alignment the\_alignment;

unsigned long num_rows();	// number of aligned	
unsigned long num_columns();	// objects. Delegate // Delegate to Alignment	
string get_name(in unsigned long row) raises(IndexOutOfBounds); StringList get_all_names();	// first object is in row // one etc // all the Names	
string get_cell_contents(in unsigned long row, in unsigned long col) raises(IndexOutOfBounds); boolean is_cell_a_gap(in unsigned long row, in unsigned long col)		
raises(IndexOutOfBounds); unsigned long get_cell_width(in unsigned lo raises(IndexOutOfBounds);	ng row, in unsigned long col)	
unsigned long max_column_width(in unsigned long col) raises(IndexOutOfBounds);		
unsigned long max_width();		

readonly attribute Alignment the_alignment;	
Description:	Provides access to the underlying <b>Alignment</b> .
Return value:	Returns an Alignment.

unsigned long num_rows();	
Description:	Provides access to the number of rows (AlignmentElements) in this Alignment. The return value of num_rows() is the same as that of the Alignment's num_rows().
Return value:	Returns an unsigned long.

unsigned long num_columns();	
Description:	Provides access to the total number of correspondences in this <b>Alignment</b> . The return value of <b>num_columns()</b> is the same as that of the <b>Alignment</b> 's <b>num_columns()</b> .
Return value:	Returns an <b>unsigned long</b> .

\_\_\_

};

string get_name(in unsigned long row) raises(IndexOutOfBounds);	
Description:	Provides access to the name associated with the <b>AlignmentElement</b> referenced by <b>row</b> .
Return value:	Returns a <b>string</b> .
Exceptions:	Raises IndexOutOfBounds if <b>row</b> is less than 1 or greater than the number of rows. This upper limit is returned by <b>num_rows()</b> .

StringList get_all_names();	
Description:	Provides access to the names associated with each of the <b>AlignmentElements</b> .
Return value:	Returns a StringList, one string per AlignmentElement.

string get_cell_contents(in unsigned long row, in unsigned long col) raises(IndexOutOfBounds);	
Description:	Provides access to the string associated with a single cell. The cell corresponds to the correspondence <b>col</b> in the <b>AlignmentElement</b> referenced by <b>row</b> .
Return value:	Returns a string.
Exceptions:	Raises IndexOutOfBounds if <b>row</b> is less than 1 or greater than the number of rows. This upper limit is returned by <b>num_rows()</b> .
	Also raises IndexOutOfBounds if <b>col</b> is less than 1 or greater than the number of columns. This upper limit is returned by <b>num_columns()</b> .

boolean is_cell_a_gap(in unsigned long row, in unsigned long col) raises(IndexOutOfBounds);	
Description:	Indicates if a single cell represents a gap in the alignment. The cell corresponds to the correspondence <b>col</b> in the <b>AlignmentElement</b> referenced by <b>row</b> .
Return value:	Returns a <b>boolean</b> .
Exceptions:	Raises IndexOutOfBounds if <b>row</b> is less than 1 or greater than the number of rows. This upper limit is returned by <b>num_rows()</b> . Also raises IndexOutOfBounds if <b>col</b> is less than 1 or greater than the number of columns. This upper limit is returned by <b>num_columns()</b> .

unsigned long get_cell_width (in unsigned long row, in unsigned long col) raises(IndexOutOfBounds);	
Description:	To allow the client to format the resulting data, <b>get_cell_width()</b> returns the width of a single cell. The cell corresponds to the correspondence <b>col</b> in the <b>AlignmentElement</b> referenced by <b>row</b> .
Return value:	Returns an <b>unsigned long</b> .
Exceptions:	Raises IndexOutOfBounds if row is less than 1 or greater than the number of rows. This upper limit is returned by num_rows(). Also raises IndexOutOfBounds if col is less than 1 or greater than the number of columns. This upper limit is returned by num_columns().

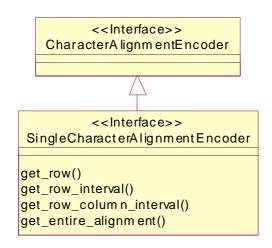
unsigned long max_column_width(in unsigned long col) raises(IndexOutOfBounds);	
Description:	To allow the client to format the resulting data, max_column_width() returns the maximum length of characters in a column defined by col.
Return value:	Returns an <b>unsigned long</b> .
Exceptions:	Raises IndexOutOfBounds if <b>col</b> is less than 1 or greater than the number of columns. This upper limit is returned by <b>num_columns()</b> .

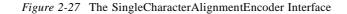
unsigned long max_width();	
Description:	To allow the client to format the resulting data, <b>max_width()</b> returns the maximum length of characters in the widest column.
Return value:	Returns an unsigned long.

## 2.1.27 SingleCharacterAlignmentEncoder (Optional)

A **SingleCharacterAlignmentEncoder** is one in which each correspondence is guaranteed to have only a single character for all **AlignmentElements**. Therefore, more bulk transport mechanisms can be employed, using strings to get rows of the **Alignment** or the entire **Alignment** as a block of text.

**SingleCharacterAlignmentEncoder** is an optional compliance point of this specification.





interface SingleCharacterAlignmentEncoder : CharacterAlignmentEncoder

string	get_row(in unsigned long row	/)
	raises(IndexOutOfBounds	5);
string	get_row_interval(in unsigned	long row, in Interval cols)
	raises(IndexOutOfBounds	s, IntervalOutOfBounds,
	SeqRegionInvalid);	
StringList	get_row_column_interval(in In	nterval rows, in Interval cols)
	raises(IntervalOutOfBoun	ds, SeqRegionInvalid);
StringList	get_entire_alignment();	// probably the most common!
	string StringList	raises(IndexOutOfBounds string get_row_interval(in unsigned raises(IndexOutOfBounds SeqRegionInvalid); StringList get_row_column_interval(in In raises(IntervalOutOfBounds

string get_row(in unsigned long row) raises(IndexOutOfBounds);	
Description:	Provides the text for all of a single <b>AlignmentElement</b> as a <b>string</b> . <b>row</b> identifies the <b>AlignmentElement</b> . There is one character per cell.
Return value:	Returns a <b>string</b> .
Exceptions:	Raises IndexOutOfBounds if <b>row</b> is less than 1 or greater than the number of rows. This upper limit is returned by <b>num_rows()</b> , inherited from <b>CharacterAlignmentEncoder</b> .

string get_row_interval(in unsigned long row, in Interval cols) raises(IndexOutOfBounds, IntervalOutOfBounds, SeqRegionInvalid);	
Description:	Provides the text for part of a single <b>AlignmentElement</b> as a <b>string</b> . <b>row</b> identifies the <b>AlignmentElement</b> . <b>cols</b> allows a subset of the correspondences to be referenced. There is one character per cell.
Return value:	Returns a <b>string</b> .
Exceptions:	Raises IndexOutOfBounds if row is less than 1 or greater than the number of rows. This upper limit is returned by num_rows(), inherited from CharacterAlignmentEncoder.Raises IntervalOutOfBounds if cols' start is less than 1 or 
	Raises SeqRegionInvalid if the interval is an invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

I

2

I

\_\_\_\_\_

StringList get_row_column_interval(in Interval rows, in Interval cols) raises(IntervalOutOfBounds, SeqRegionInvalid);	
Description:	Provides the sub-block of text for the portion of the Alignment defined by rows and cols Intervals as an array of strings. rows allows a subset of the AlignmentElements to be referenced. cols allows a subset of the correspondences to be referenced. There is one character per cell.
Return value:	Returns a <b>StringList</b> , one <b>string</b> per row.
Exceptions:	Raises IntervalOutOfBounds if rows' start is less than 1 or start+length-1 is greater than the number of rows. This upper limit is returned by num_rows(), inherited from CharacterAlignmentEncoder.
	than 1 or <b>start+length-1</b> is greater than the number of columns. This upper limit is returned by <b>num_cols()</b> , inherited from <b>CharacterAlignmentEncoder</b> .
	Raises SeqRegionInvalid if the interval is an invalid SeqRegion. Examples include an incorrect StrandType, or an invalid CompositeSeqRegion (e.g., one that has a wrong SeqRegionOperator or contains overlaps or circularities).

StringList get_entire_alignment();	
Description:	Provides the block of text for the entire <b>Alignment</b> as an array of <b>strings</b> . There is one character per cell.
Return value:	Returns a StringList, one string per row.

## 2.1.28 AlignmentEncoder factories (Optional)

AlignmentEncoder factories provide a means of creating new CharacterAlignmentEncoder and SingleCharacterAlignmentEncoder objects. This permits a clean separation of factory issues from the AlignmentEncoder objects themselves.

AlignmentEncoder factories are an optional compliance point of this specification.

< <interface>&gt; CharacterAlignmentEncoderFactory</interface>
create()

< <interface>&gt;</interface>
SingleCharacterAlignmentEncoderFactory
create()



## **CannotEncodeAlignment**

exception CannotEncodeAlignment {     string reason; };	
Description:	The CannotEncodeAlignment exception is raised if an <b>AlignmentEncoder</b> can not be created for this <b>Alignment</b> .
Return value:	Returns a <b>string</b> containing the reason the <b>AlignmentEncoder</b> could not be created for this <b>Alignment</b> .

### CharacterAlignmentEncoderFactory

CharacterAlignmentEncoderFactory provides a means of creating new CharacterAlignmentEncoders for an Alignment.

**CharacterAlignmentEncoderFactory** is an optional compliance point of this specification.

```
interface CharacterAlignmentEncoderFactory
```

{

CharacterAlignmentEncoder create(in Alignment the\_alignment) raises(CannotEncodeAlignment);

};

CharacterAlignmentEncoder create(in Alignment the_alignment) raises(CannotEncodeAlignment);	
Description:	The create() operation creates a CharacterAlignmentEncoder for the given Alignment.
Return value:	Returns a CharacterAlignmentEncoder.
Exceptions:	Raises CannotEncodeAlignment if a CharacterAlignmentEncoder cannot be created for this Alignment.

#### SingleCharacterAlignmentEncoderFactory

SingleCharacterAlignmentEncoderFactory provides a means of creating new SingleCharacterAlignmentEncoders for an Alignment.

**SingleCharacterAlignmentEncoderFactory** is an optional compliance point of this specification.

interface SingleCharacterAlignmentEncoderFactory

- {
- SingleCharacterAlignmentEncoder create(in Alignment the\_alignment) raises(CannotEncodeAlignment);
- };

SingleCharacterAlignmentEncoder create(in Alignment the_alignment) raises(CannotEncodeAlignment);	
Description:	The <b>create</b> () operation creates a <b>SingleCharacterAlignmentEncoder</b> for the given <b>Alignment</b> .
Return value:	Returns a SingleCharacterAlignmentEncoder.
Exceptions:	Raises CannotEncodeAlignment if a SingleCharacterAlignmentEncoder cannot be created for this Alignment.

# 2.2 Module DsLSRAnalysis

The **DsLSRAnalysis** module defines the component interfaces for supporting sequence analysis through a generic analysis design. The module encapsulates the required elements for analysis. It provides the means to interrogate analyses inputs, output and functionality. An analysis can be executed asynchronously as well as synchronously based on the client invocation. Executing analyses can be monitored by subscribing to an event channel or polling for state.

The Client is responsible for:

- determining which Biomolecular Sequence Analysis (BSA) analysis tool (e.g., BLAST, Smith-Waterman, etc.) it wants to employ;
- locating an **AnalysisService** that represent the BSA analysis tool;
- retrieving a handle to an **AnalysisInstance** object that implements the BSA analysis tool;
- providing the **AnalysisInstance** with complete input information;
- invoking the **AnalysisInstance** to perform its function (via a synchronous or asynchronous mechanism);
- retrieving results generated by the BSA analysis tool execution; and
- when it no longer requires an **AnalysisInstance** (and its related input and output objects), invoking their removal from the system.

A Client can learn about processing events that occur during the execution of an **AnalysisInstance** either by asking the **AnalysisInstance** for its most recent processing event or listening to an event channel on which the **AnalysisInstance** publishes its events. A Client can also ask for an **AnalysisInstance**'s execution status.

## 2.2.1 General

//File: DsLSRAnalysis

#ifndef \_DS\_LSR\_ANALYSIS\_IDL\_
#define \_DS\_LSR\_ANALYSIS\_IDL\_

#pragma prefix "omg.org"

#include <orb.idl>
#include <CosPropertyService.idl>
#include <CosEventChannelAdmin.idl>
#include <CosLifeCycle.idl>
#include <TimeBase.idl>

module DsLSRAnalysis

{ // ... };

```
#endif // _DS_LSR_ANALYSIS_IDL_
```

## #pragma prefix ''omg.org''

To prevent name pollution and name clashing of IDL types, this module (and all modules defined in this specification) uses the pragma prefix that is the OMG's DNS name.

#### #include <orb.idl>

CORBA::TypeCode is used in InputPropertySpec and OutputPropertySpec.

*#include <CosPropertyService.idl>* 

Properties are used in AnalysisService and AnalysisInstance.

#include <CosEventChannelAdmin.idl>

EventChannel is used in AnalysisInstance.

#include <CosLifeCycle.idl>

AnalysisInstance inherits from LifeCycleObject.

I

#### #include <TimeBase.idl>

TimeT is used in TimeProgressEvent and JobControl. UtcT is used in JobControl.

#### **StringList**

typedef sequence <string> StringList;</string>	
Description:	Used to pass and return a set of <b>strings</b> .

## 2.2.2 AnalysisType

An **AnalysisType** provides information for a client to determine the types of BSA analyses available in the system. It can also be used to distinguish the type of analysis offered by an **AnalysisService**. An **AnalysisType** provides information sufficient to determine whether two **AnalysisServices** create identical BSA **AnalysisInstances**. Such information may be of use to a computation management subsystem such as a load balancing or queuing system. To provide enough information to distinguish analysis types, there are several attributes of an **AnalysisType**.

It is important to note that the **AnalysisType** is defined as a **valuetype** that can be extended by a vendor requiring additional attributes.

< <valuetype>&gt; AnalysisType</valuetype>
type : string name : string supplier : string version : string installation : string description : string

Figure 2-29 The AnalysisType valuetype

```
valuetype AnalysisType
{
    public string type;
    public string name;
    public string supplier;
    public string version;
    public string installation;
    public string description;
};
```

public string type;	
Description:	The <b>type</b> attribute is used to specify both the correct classification of the analysis as well as a qualifier to specify category and additionally, provides information about the inputs to the analysis. The classification of the analysis could come from the BSA specified classification hierarchy as well as it could come from a hierarchy defined by a certain installation. A '/' is used to delimit the qualifier and a '.' is used to delimit the general input kind. An example of a specified <b>type</b> attribute would be <i>alignment.collection/assembly</i> .
Return value:	Returns a <b>string</b> .

public string name;	
Description:	The <b>name</b> attribute is used to further identify the analysis in the system.
Return value:	Returns a <b>string</b> .

public string supplier;	
Description:	The <b>supplier</b> attribute is used to identify the supplier or vendor of a custom analysis implementation.
Return value:	Returns a <b>string</b> .

public string version;	
Description:	The <b>version</b> attribute specifies the particular form or variation of the analysis.
Return value:	Returns a <b>string</b> .

public string installation;		
Description:	The <b>installation</b> attribute is used to differentiate similar analysis implementations at a particular installation.	
Return value:	Returns a string.	

public string description;	
Description: The <b>description</b> attribute is used to provide useful descriptive information about the <b>AnalysisInstances</b> created by the <b>AnalysisService</b> .	
Return value:	Returns a <b>string</b> .

## 2.2.3 InputPropertySpec

An **InputPropertySpec** is used to provide metadata that describes required and optional input parameters used to perform an analysis. The **InputPropertySpec** provides an input name and **CORBA::TypeCode** to allow the client to interrogate the interface repository for more information about the analysis parameter. Additionally, there are some useful attributes that help the client determine if a parameter is optional or required, the default value of an input parameter if one exists, and finally some possible values useful for validation or user-interface presentation.

< <valuetype>&gt; InputPropertySpec</valuetype>
name : string type : CORBA::TypeCode mandatory : boolean default_value : any possible_values : any

Figure 2-30 The InputPropertySpec valuetype

#### InputPropertySpec

valuetype InputPropertySpec

public string	name;
public CORBA::TypeCode	type;
public boolean	mandatory;
public any	default_value;
public any	possible_values;

};

{

public string name;	
Description:	This is the name of the parameter that can be submitted to initialize the analysis.
Return value:	Returns a string.

public CORBA::TypeCode type;	
Description:	This is a <b>CORBA::TypeCode</b> allowing the client to find more detailed information in the interface repository about the data type.
Return value:	Returns a CORBA::TypeCode.

public boolean mandatory;	
Description:	The <b>mandatory</b> attribute specifies if the analysis requires the parameter with TRUE and if the parameter is optional with FALSE.
Return value:	Returns a <b>boolean</b> .

public any default_value;	
Description:	This attribute specifies the default value if one is applicable. If no default value is applicable, return a null in the <b>any</b> .
Return value:	Returns a CORBA <b>any</b> .

public any possible_values;	
Description:	This attribute specifies suggested allowed values that are applicable. If no possible values are applicable, return a null in the <b>any</b> .
Return value:	Returns a CORBA <b>any</b> .

## InputPropertySpecList

typedef sequence <inputpropertyspec> InputPropertySpecList;</inputpropertyspec>	
Description:	Used to pass a set of InputPropertySpecs.

# 2.2.4 OutputPropertySpec

An **OutputPropertySpec** is used to provide metadata that describes each output value generated by an analysis. The **OutputPropertySpec** provides an output argument **name** and **CORBA::TypeCode** to allow the client to interrogate the interface repository for more information about the output value.

< <valuetype>&gt; OutputPropertySpec</valuetype>
name : string type : CORBA::TypeCode

Figure 2-31 The OutputPropertySpec valuetype

## **OutputPropertySpec**

valuetype OutputPropertySpec
{
 public string name;
 public CORBA::TypeCode type;
};

public string name;	
Description:	This is the name of the identifier that contains an analysis output value.
Return value:	Returns a <b>string</b> .

public CORBA::TypeCode type;	
Description:	This is a <b>CORBA::TypeCode</b> allowing the client to find more detailed information in the interface repository about the data type.
Return value:	Returns a CORBA::TypeCode.

#### **OutputPropertySpecList**

typedef sequence<OutputPropertySpec> OutputPropertySpecList;Description:Used to pass a set of OutputPropertySpecs.

## 2.2.5 AnalysisState

There are five defined analysis states:

- 1. CREATED created but not yet invoked.
- 2. RUNNING invoked.
- 3. **COMPLETED** execution ended normally.
- 4. TERMINATED\_BY\_REQUEST execution was terminated by a user request.
- 5. **TERMINATED\_BY\_ERROR** execution terminated abnormally.

When an **AnalysisInstance** is first created it will be in the **CREATED** state. When the **AnalysisInstance** is successfully **run()** it will move into the **Running** state. In due course, the **AnalysisInstance** will then enter *either* the **COMPLETED**, **TERMINATED\_BY\_REQUEST** *or* **TERMINATED\_BY\_ERROR** state.

Note that an **AnalysisInstance** in the **TERMINATED\_BY\_REQUEST** or **TERMINATED\_BY\_ERROR** states may still have (partial, incomplete) results that can be retrieved by the client. There is no obligation that an implementation provides results in these two cases. Further, the results for an analysis that is in one of these two states is likely to be different than for an analysis that ran to normal completion. It is recommended that client software convey this information to the end-user.

< <enum>&gt;</enum>
AnalysisState
CREATED
RUNNING
COMPLETED
TERMINATED_BY_REQUEST
TERMINATED_BY_ERROR

Figure 2-32 The AnalysisState enumeration

#### enum AnalysisState

٤		
	CREATED,	// Instance has been created but not yet executed.
	RUNNING,	// The analysis instance is running.
	COMPLETED,	// The instance has completed execution.
	TERMINATED_BY_REQUES	Γ,// The instance was terminated by user request.
	TERMINATED_BY_ERROR	// The instance terminated due to an error.
};		

CREATED	<b>CREATED</b> should be used when the <b>AnalysisInstance</b> has been created but not yet invoked.
RUNNING	<b>RUNNING</b> should be used when the <b>AnalysisInstance</b> has been invoked.
COMPLETED	<b>COMPLETED</b> should be used to indicate that the execution of the <b>AnalysisInstance</b> ended normally.
TERMINATED_BY_REQUEST	<b>TERMINATED_BY_REQUEST</b> should be used to indicate that the execution of the <b>AnalysisInstance</b> was terminated by a user request.
TERMINATED_BY_ERROR	<b>TERMINATED_BY_ERROR</b> should be to indicate that the execution of the <b>AnalysisInstance</b> was terminated abnormally.

## 2.2.6 AnalysisEvent

There are five defined types of analysis events. They all inherit from the base valuetype, which has a single message string. For all events the string should give some free-form text description of the current progress.

- StateChangedEvent
- HeartbeatProgressEvent
- PercentProgressEvent
- StepProgressEvent
- TimeProgressEvent

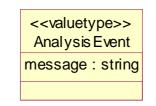


Figure 2-33 The AnalysisEvent valuetype

valuetype AnalysisEvent

{ public string message;

};

public string message;	
Description:	For all events <b>message</b> should give some free-form text description of the current progress.
Return value:	Returns a <b>string</b> .

### 2.2.7 Sub-types of AnalysisEvent

If an analysis has a non-null event channel then it must publish **StateChangedEvents** onto that channel whenever the analysis enters a new state (apart from the **CREATED**) state.

The frequency of publication of other events onto the event channel is considered a quality of implementation issue. There is no restriction on the ordering of the events published onto the event channel.

An analysis may also publish other events (not necessarily derived from **AnalysisEvent**) onto the event channel. Clients, therefore, must be capable of dealing with unknown events (e.g. by discarding them).

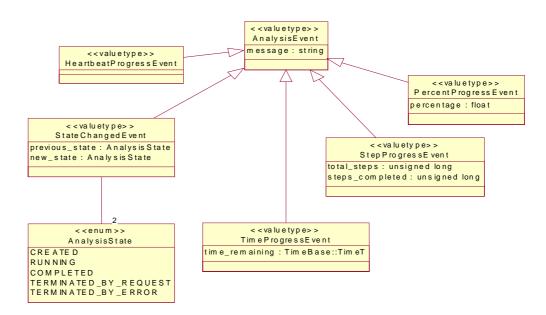


Figure 2-34 The Sub-types of AnalysisEvent

#### StateChangedEvent

StateChangedEvent indicates that an AnalysisInstance has changed from one of the five defined AnalysisStates to another. StateChangedEvent is truncatable to AnalysisEvent.

If an analysis has a non-null event channel then it must publish **StateChangedEvents** onto that channel whenever the analysis enters a new state (apart from the **CREATED**) state.

valuetype StateChangedEvent : truncatable AnalysisEvent
{
 public AnalysisState previous\_state;
 public AnalysisState new\_state;

};

1

public AnalysisState previous_state;	
Description:	Provides the previous state of the <b>AnalysisInstance</b> .
Return value:	Returns an AnalysisState.

public AnalysisState new_state;	
Description:	Provides the new state of the <b>AnalysisInstance</b> .
Return value:	Returns an AnalysisState.

#### *HeartbeatProgressEvent*

HeartbeatProgressEvent indicates that an AnalysisInstance is still alive and running. HeartbeatProgressEvent is truncatable to AnalysisEvent.

valuetype HeartbeatProgressEvent : truncatable AnalysisEvent

{ };

#### **PercentProgressEvent**

**PercentProgressEvent** provides information regarding the relative amount of work completed by an **AnalysisInstance** in terms of percentage complete. The percentage parameter must be greater or equal to 0 and less than or equal to 100. **PercentProgressEvent** is truncatable to **AnalysisEvent**.

#### valuetype PercentProgressEvent : truncatable AnalysisEvent

{

public float percentage;

};

public float percentage;	
Description:	<b>percentage</b> must be greater or equal to 0 and less than or equal to 100.
Return value:	Returns a <b>float</b> .

#### **TimeProgressEvent**

**TimeProgressEvent** indicates the estimated completion time relative to the current time. There is no requirement that the estimated completion time decreases! **TimeProgressEvent** is truncatable to **AnalysisEvent**.

valuetype TimeProgressEvent : truncatable AnalysisEvent

public TimeBase::TimeT time\_remaining;

};

{

public TimeBase::TimeT time_remaining;	
Description:	Indicates the estimated completion time relative to the current time.
Return value:	Returns a TimeBase::TimeT.

### **StepProgressEvent**

StepProgressEvent indicates the total number of steps to be executed by an AnalysisInstance and the number of steps completed so far. Multiple StepProgressEvents with the same progress string must have the same total number of steps. The steps\_completed parameter must be less than or equal to the total\_steps parameter. StepProgressEvent is truncatable to AnalysisEvent.

valuetype StepProgressEvent : truncatable AnalysisEvent {

public unsigned long total\_steps; public unsigned long steps\_completed;

**}**;

public unsigned long total_steps;	
Description:	Indicates the total number of steps to be executed by the <b>AnalysisInstance</b> . The <b>steps_completed</b> parameter must be less than or equal to the <b>total_steps</b> parameter.
Return value:	Returns an unsigned long.

public unsigned long steps_completed;	
Description:	Indicates the number of steps completed so far. The <b>steps_completed</b> parameter must be less than or equal to the <b>total_steps</b> parameter.
Return value:	Returns an unsigned long.

#### 2.2.8 AnalysisService

I

An **AnalysisService** is a logical representation of a particular type of a BSA analysis tool available within a system. An **AnalysisService** provides enough information to distinguish the service it provides from those offered by other **AnalysisServices**.

An **AnalysisService** provides metadata that describes input to its **AnalysisInstances** and the output generated by its **AnalysisInstances**. Metadata describing input and output parameters is available to the client in either IDL valuetypes or both IDL valuetypes and XML strings. If both are used, the information available in the IDL structures and XML strings must not be contradictory. Obviously there is some information, such as constraints expressed in OCL (Object Constraint Language), that will only be available in the XML strings. Metadata is required for a compliant implementation.

An **AnalysisService** creates and returns references to **AnalysisInstance** objects that implement the BSA analysis tool it represents. Arguments to create an **AnalysisInstance** are in the form of **CosPropertyService::Properties**. Before returning an **AnalysisInstance**, the input arguments must be checked for correctness (according to the criteria represented in the metadata describing the **AnalysisService's** input parameters).

The client that receives the returned reference to an **AnalysisInstance** is responsible for the lifecycle management of that instance along with the objects populating the **AnalysisInstance's** input parameters and output parameters.

< <interface>&gt;</interface>		
AnalysisService		
AnalysisTypeTag : string = "TAG_ANALYSIS_TYPE"		
InputPropertiesTag : string = "TAG_INPUT_PROPERTIES"		
OutputPropertiesTag : string = "TAG_OUTPUT_PROPERTIES"		
metadata_tags : StringList		
type : AnalysisType		
input_metadata : InputPropertySpecList		
output_metadata : OutputPropertySpecList		
create_analysis()		
describe()		

Figure 2-35 The AnalysisService interface

#### MetaData

typedef string MetaData;	
Description:	Used to pass and return a string containing XML metadata.

#### **DoesNotExistException**

exception DoesNotExistException { };	
Description:	The DoesNotExistException exception is raised if the
	tagname used in describe() does not exist in the metadata.

#### **AnalysisService**

#### interface AnalysisService

{

const string AnalysisTypeTag	= "TAG_ANALYSIS_TYPE";
const string InputPropertiesTag	= "TAG_INPUT_PROPERTIES";
const string OutputPropertiesTag	= "TAG_OUTPUT_PROPERTIES";

readonly attribute StringList metadata\_tags; MetaData describe(in string tagname) raises (DoesNotExistException);

readonly attribute AnalysisType type; readonly attribute InputPropertySpecList input\_metadata; readonly attribute OutputPropertySpecList output\_metadata;

AnalysisInstance create\_analysis (in CosPropertyService::Properties input) raises (CosPropertyService::MultipleExceptions);

};

const string AnalysisTypeTag = "TAG_ANALYSIS_TYPE"; const string InputPropertiesTag = "TAG_INPUT_PROPERTIES"; const string OutputPropertiesTag = "TAG_OUTPUT_PROPERTIES";	
Description:	The <b>AnalysisService</b> interface defines a set of <b>const</b> <b>strings</b> that indicates the types of required metadata. The strings correspond to the three attributes described below.

readonly attribute StringList metadata_tags;	
Description:	Provides the set of metadata tags for this analysis. The list must include the three <b>const strings</b> listed above.
Return value:	Returns a StringList.

MetaData describe(in string tagname) raises (DoesNotExistException);	
Description:	<b>describe()</b> returns an XML string containing the metadata corresponding to the tagname parameter. If metadata is available as XML, <b>describe()</b> must support all tagnames returned by the metadata_tags attribute.
Return value:	Returns a MetaData string containing XML.
Exceptions:	Raises DoesNotExistException if the tagname parameter is not one of the list returned by the metadata_tags attribute. Raises CORBA::NO_IMPLEMENT with standard minor code 6 if metadata is not available as XML.

readonly attribute AnalysisType type;	
Description:	<b>type()</b> returns the <b>AnalysisType</b> structure. This structure must be populated.
Return value:	Returns an AnalysisType.

readonly attribute InputPropertySpecList input_metadata;	
Description:	<b>input_metadata()</b> returns information about input parameters in IDL structure form. This structure must be populated.
Return value:	Returns an array of InputPropertySpecs.

readonly attribute OutputPropertySpecList output_metadata;	
Description:	<b>output_metadata()</b> returns information about output parameters in IDL structure form. This structure must be populated.
Return value:	Returns an array of <b>OutputPropertySpecs</b> .

AnalysisInstance create_analysis (in CosPropertyService::Properties input) raises (CosPropertyService::MultipleExceptions);	
Description:	Arguments to create an <b>AnalysisInstance</b> are in the form of <b>CosPropertyService::Properties</b> . Before returning an <b>AnalysisInstance</b> , the input arguments must be checked for correctness (according to the criteria represented in the metadata describing the <b>AnalysisService</b> 's input parameters).
Return value:	Returns an AnalysisInstance.
Exceptions:	Raises <b>CosPropertyService::MultipleExceptions</b> if the input parameters are incorrect for this analysis. The metadata should be consulted for information about the input parameters needed by this analysis.

## 2.2.9 JobControl

Along with its basic interface, an **AnalysisInstance** implements a **JobControl** interface. Via the **JobControl**, clients invoke and terminate **AnalysisInstance** execution and retrieve execution information (e.g., execution duration, creation time).

I

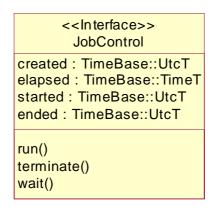


Figure 2-36 The JobControl interface

#### NotRunnable

exception NotRunnable { };	
Description:	The NotRunnable exception is raised if the analysis cannot be run (e.g., the service is currently unavailable). Raised by <b>run()</b> .
	This exception should not be used to indicate incorrect inputs. <b>CosPropertyService::MultipleExceptions</b> should be used instead.

## NotRunning

exception NotRunning { };	
-	The NotRunning exception is raised if the analysis is not running. Raised by <b>terminate()</b> .

### NotTerminated

exception NotTerminated { string reason; };	
Description:	The NotTerminated exception is raised if the analysis is not terminated. Raised by <b>terminate()</b> .
Return value:	Returns a <b>string</b> containing the reason the analysis could not be terminated.

{

interface JobControl

readonly attribute TimeBase::UtcT created; readonly attribute TimeBase::TimeT elapsed; readonly attribute TimeBase::UtcT started; readonly attribute TimeBase::UtcT ended;

void run()

raises (NotRunnable, CosPropertyService::MultipleExceptions);

void terminate() raises (NotRunning, NotRunnable, NotTerminated);

```
void wait()
```

raises (NotRunning, NotRunnable);

};

readonly attribute TimeBase::UtcT created;	
Description:	Indicates the time the <b>AnalysisInstance</b> was created.
Return value:	Returns a TimeBase::UtcT.

readonly attribute TimeBase::TimeT elapsed;	
Description:	Indicates the elapsed time since the analysis was started using <b>run()</b> .
Return value:	Returns a TimeBase::TimeT.

readonly attribute TimeBase::UtcT started;			
Description:	ption: Indicates the time the analysis was started.		
Return value: Returns a <b>TimeBase::UtcT</b> .			

readonly attribute TimeBase::UtcT ended;		
Description:	Description: Indicates the time the analysis ended.	
Return value:	eturn value: Returns a <b>TimeBase::UtcT</b> .	

I

void run() raises (NotRunnable, CosPropertyService::MultipleExceptions);		
Description:	The <b>run()</b> method invokes the <b>AnalysisInstance</b> to run asynchronously	
Exceptions:	Raises NotRunnable if the analysis cannot be run (e.g., the service is currently unavailable).	
	Raises CosPropertyService::MultipleExceptions if the inputs are not correct.	

void terminate() raises (NotRunning, NotRunnable, NotTerminated);			
Description:	terminate() ends a currently running analysis.		
Exceptions:	Raises NotRunning if the analysis is not running.		
	Raises NotRunnable if the analysis cannot be run (e.g., the has already completed or terminated).		
	Raises NotTerminated if the analysis was not terminated.		

void wait() raises (NotRunning, NotRunnable);	
Description:	The <b>wait()</b> method blocks the client until service execution completes.
Exceptions:	Raises NotRunning if the analysis is not running. Raises NotRunnable if the analysis cannot be run (e.g., the has been terminated).

The following table summarizes the behavior of the three methods for each possible state of the **AnalysisInstance**.

Table 2-7         JobControl State Transition Table	Table 2-7	JobControl State Transition Table
---	-----------	-----------------------------------

I

State of AnalysisInstance	run()	wait()	terminate()
CREATED	start it and change status to <b>RUNNING</b>	raise NotRunning	raise NotRunning

2		

State of AnalysisInstance	run()	wait()	terminate()
RUNNING	raise NotRunnable	block until finished	kill it and change status to TERMINATED_BY_ REQUEST or raise NotTerminated
COMPLETED	raise NotRunnable	do nothing	raise NotRunnable
TERMINATED_BY_REQUEST	raise NotRunnable	raise NotRunnable	raise NotRunnable
TERMINATED_BY_ERROR	raise NotRunnable	raise NotRunnable	raise NotRunnable

Table 2-7 JobControl State Transition Table

### 2.2.10 AnalysisInstance

An **AnalysisInstance** object is responsible for invoking an underlying BSA analysis tool.

An **AnalysisInstance** can be used in either a synchronous or an asynchronous mode to support clients with various needs. The **run()** method invokes the **AnalysisInstance** to run asynchronously. If the client wants to be blocked waiting for the underlying BSA analysis tool to run to completion, it will invoke the **run()** method, followed immediately by the **wait()** method, which will block the client until service execution completes.

An **AnalysisInstance** must ensure it can be executed only once, ensuring a unique coupling of inputs and results. If a client wants to employ an **AnalysisInstance** identical to one it has already invoked, the client must create a new **AnalysisInstance**, via an **AnalysisService**, and invoke it as a separate instance.

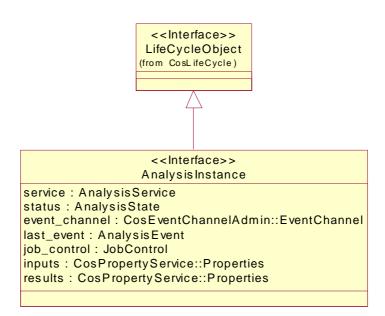
An **AnalysisInstance** makes available two kinds of execution information: execution status and analysis events.

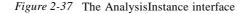
- An AnalysisInstance object must offer:
  - the AnalysisService that created this AnalysisInstance;
  - its execution status (one of the enumerated AnalysisState values);
  - the **EventChannel**, which may be null, to which it publishes its analysis events;
  - the last event that occurred;
  - the **JobControl** that clients use to control the execution;
  - the input **Properties** used in creation of this **AnalysisInstance**;
  - an output **Properties** containing the results generated by the execution of the underlying BSA analysis.

An **AnalysisInstance** is responsible for ensuring that the results of the BSA analysis tool it represents are populated properly in its **results**.

To retrieve the results generated by an **AnalysisInstance**, clients use the **get\_result()** method. It takes a list of strings (the strings representing named members of the **OutputPropertySpecList**) as an argument. If the BSA analysis tool underlying the **AnalysisInstance** terminated before it completed, either due to a client request or an execution failure, some "partial" results may be available to the client in the **results**.

As in all CORBA systems, an implementation of this system may choose to enforce a policy regarding automatically removing CORBA objects, such as **AnalysisInstances** that appear to have been abandoned by clients.





interface AnalysisInstance : CosLifeCycle::LifeCycleObject
{

- readonly attribute AnalysisService service; readonly attribute AnalysisState status; readonly attribute CosEventChannelAdmin::EventChannel event\_channel; readonly attribute AnalysisEvent last\_event; readonly attribute JobControl job\_control; readonly attribute CosPropertyService::Properties inputs; readonly attribute CosPropertyService::Properties results; CosPropertyService::Properties get\_result(in StringList name\_list);
- };

readonly attribute AnalysisService service;		
Description:	Refers to the <b>AnalysisService</b> that created this <b>AnalysisInstance</b> .	
Return value:	Returns an AnalysisService.	
Exceptions:	Raises CORBA::OBJECT_NOT_EXIST with standard minor code 3 if the <b>AnalysisService</b> is no longer available.	

readonly attribute AnalysisState status;	
Description:	Provides the current status of the analysis.
Return value:	Returns one of the enumerated <b>AnalysisState</b> values. The values are <b>CREATED</b> , <b>RUNNING</b> , <b>COMPLETED</b> , <b>TERMINATED_BY_REQUEST</b> , and <b>TERMINATED_BY_ERROR</b> .

readonly attribute CosEventChannelAdmin::EventChannel event_channel;		
Description:	Description: Provides the <b>EventChannel</b> to which the <b>AnalysisInstance</b> publishes its analysis events.	
Return value:	Returns a CosEventChannelAdmin::EventChannel.	

readonly attribute AnalysisEvent last_event;			
Description:	Provides the last event that occurred during execution. If the <b>AnalysisInstance</b> is still in the <b>CREATED</b> state, the <b>last_event</b> should be a plain <b>AnalysisEvent</b> .		
Return value:	Returns an AnalysisEvent.		

readonly attribute JobControl job_control;		
Description:	Provides the management interface that clients can use to control the execution of the analysis.	
Return value:	Returns a <b>JobControl</b> .	

readonly attribute CosPropertyService::Properties inputs;		
Description:	Provides the input <b>Properties</b> that were used in this <b>AnalysisInstance</b> 's execution.	
Return value:	Returns a CosPropertyService::Properties.	

readonly attribu	ute CosPropertyService::Properties results;
Description:	Provides the output <b>Properties</b> containing the results generated by the execution of the underlying BSA analysis.
	Note 1: An AnalysisInstance in the RUNNING or TERMINATED_BY_REQUEST or
	<b>TERMINATED_BY_ERROR</b> states may still have (partial, incomplete) results that can be retrieved by the client. There is no obligation that an implementation provides results in these three cases. Further, the results for an analysis that is in one of these three states is likely to be different than for an analysis that ran to normal completion. It is recommended that client software convey this information to the end-user.
	Note 2: An <b>AnalysisInstance</b> in the <b>CREATED</b> state returns an empty list of results.
Return value:	Returns a CosPropertyService::Properties.

I

CosPropertySe	ervice::Properties get_result(in StringList name_list);
Description:	The <b>get_result()</b> method takes a list of strings (the strings representing named members of the <b>OutputPropertySpecList</b> ) as an argument and returns the associated results.
	Note 1: An <b>AnalysisInstance</b> in the <b>RUNNING</b> or <b>TERMINATED_BY_REQUEST</b> or <b>TERMINATED_BY_ERROR</b> states may still have (partial, incomplete) results that can be retrieved by the client. There is no obligation that an implementation provides results in these three cases. Further, the results for an analysis that is in one of these three states is likely to be different than for an analysis that ran to normal completion. It is recommended that client software convey this information to the end-user. Note 2: An <b>AnalysisInstance</b> in the <b>CREATED</b> state
Return value:	returns an empty list of results.         Returns a CosPropertyService::Properties.

### 2.2.11 Sequence Diagrams

The following sequence diagrams show how the analysis machinery is used. The diagrams are examples of the steps necessary for both synchronous and asynchronous invocation of an analysis service and retrieving its results.

Synchronous invocation can be achieved without using any **EventChannel** interface. The client is blocked in **wait()** method until the analysis is finished.

Asynchronous invocation, using an **EventChannel**, can follow a "callback" pattern where the server regularly pushes events back to an object prepared by the client, or the client can repeatedly poll the server.

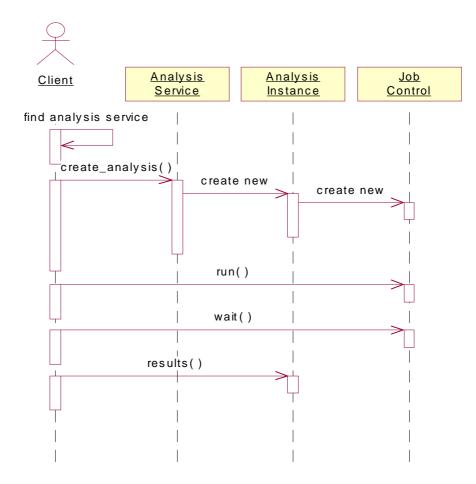


Figure 2-38 Synchronous invocation without using an EventChannel

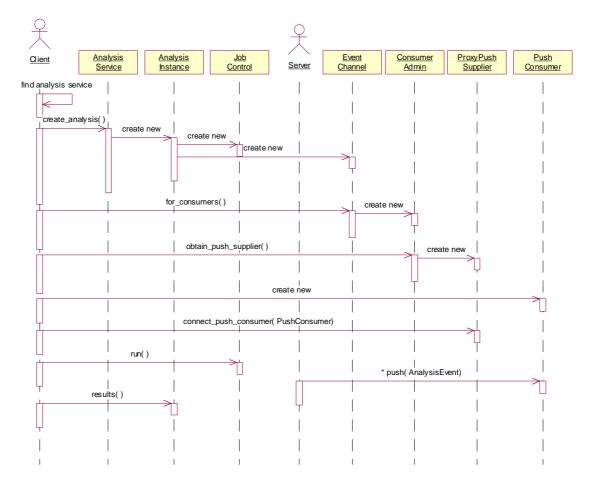


Figure 2-39 Asynchronous invocation, using an EventChannel and callbacks

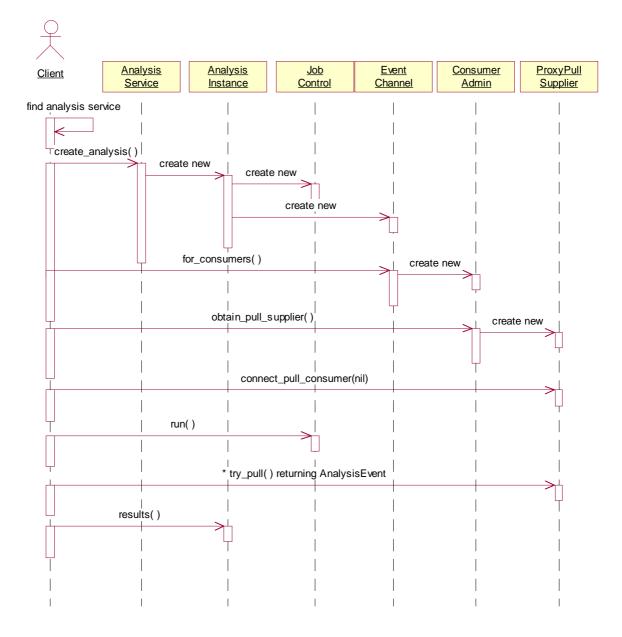


Figure 2-40 Asynchronous invocation, using an EventChannel and polling

# Domain Model

### Contents

This chapter contains the following sections.

Section Title	Page
"XML Metadata"	3-1
"Classification of Analyses"	3-6

The domain model is expressed in XML. A simple classification of analyses follows the explanation of XML metadata. The DTD and the entire XML file can be found in Appendix D.

## 3.1 XML Metadata

Metadata is used in the **AnalysisService** for analysis type, input and output objects to represent object implementation detail that has been abstracted out of the interface in favor of using the standard, common BSA analysis interface. This can provide semantic information beyond that provided by the IDL syntax, although information provided through XML must not be contradictory with information available through IDL structures. XML has been chosen as the language with which to represent the object metadata. This section discusses the strategy for using the XML based metadata representation.

### 3.1.1 Role of XML

"Standard Generalized Markup Language (SGML), which became an ISO 8879 standard in 1986, was the result of a decade's long effort to produce a language for writing human consumable text that at the same time is machine processable. Hypertext Markup Language (HTML), a limited subset of SGML, is one of the driving forces behind the success of the internet. HTML is non-extensible and primarily designed to support rendering in a browser and a limited amount of user interaction. Extensible Markup Language (XML) is a larger subset of SGML which overcomes the non-extensible nature of HTML and reintroduces support for the machine processing of text via the definition of user specified tag sets. Since its inception, XML has offered the prospect of overcoming the limitations of HTML without unduly burdening development of processing software as has been the case with SGML based systems. Unlike HTML, XML does not rely on a fixed set of tags. Arbitrary tag sets can be defined via use of a DTD. However, XML eliminates several features of SGML which make it difficult to parse and therefore difficult to process SGML documents. In particular, begin and end tags are both required and serve to reduce ambiguity in the processing of the hierarchical structure of XML documents, relative to SGML documents. In short, XML provides a standardized, non-proprietary capability to represent arbitrary structural information in a way that supports development of parsers and other types of processing of that structural information. Thus, XML opens up the possibility of automated processing and interchange of information stored in the form of XML documents.

With respect to metadata, it opens up the possibility of accessing metadata at runtime and using the structural information provided by the XML based tags to process and transform that metadata. For example, the metadata for two separate processes could be used at runtime to connect the output of one process to the input of another process via conversion of the output format of the first process into the input format of the second process."

[Concept Five Technologies, Inc., *Trident Next Generation Metadata Design and Generation Manual version 1.01*, pages 3-4, Copyright © 1998, 1999 by Hitachi, Ltd. and Concept Five Technologies, Inc.]

### 3.1.2 Role of DTD

As the XML proposal most succinctly puts, "The XML document type declaration contains or points to markup declarations that provide a grammar for a class of documents. This grammar is known as a document type definition, or DTD."

The markup grammar is a generic set of keywords, naming syntax, occurrence and connector terms prescribed in the XML standard that the document structure designer wishes to use to express literally any real world semantic notion. The basic markup keywords are ELEMENT, ENTITY and ATTRIBUTE although there are dozens of others to round out the language. Any set of key words could have been chosen. Microsoft Word has its set of formatting keywords and arguments that allow a .doc file to carry a formidable amount of information around for future processing. WordPerfect used to allow a document writer to make these codes visible and directly editable at the click of a menu item. And of course, there is post script.

There are many other document code sets, all of which are proprietary. Document processing code that operates on these proprietarily marked up documents must necessarily also be proprietary. Enter the DTD, or Document Type Definition. ISO 8879 makes standard these markup codes so non-proprietary document software can be developed.

Hypertext Markup Language (HTML) is an example of a markup language. Although HTML is not based on a DTD it does adhere to a standard and stems from SGML. HTML was designed so that processing code could be developed for rendering HTML based doc-

uments in a browser. The HTML standard (currently 4.0) specifies the structure of valid HTML documents. Changing one of the tags in this standard from  $\langle H3 \rangle$  to  $\langle J3 \rangle$  has the potential to break all the processing code that relies on the use of the standard, which is why changes to HTML are only made infrequently. Recently, DTD's have been developed for HTML, but these DTD's do not adhere strictly to the standard, and are not widely used.

In general, DTD's make it possible to specify the grammars of various domains so that companies creating XML documents in these domains can interact with each other. For example, there is a DTD for the representation of chemical formulas in XML. Companies complying with the grammar for this domain can expect to be able to exchange XML documents describing chemical formulas and be able to use any processing code designed to operate in this domain. For example, processing code that accepts XML based descriptions of chemical formulas and creates graphical representations of the formulas should be able to handle any documents complying with the DTD.

At the present time, DTD's are being generated for many different domains. The Dublin Core is a DTD which provides a tag set designed for use in the description of Internet information resources and which is patterned after the information in a card catalog. The UML DTD which is derived from the XMI specification covers the domain of object modeling and is based on the UML semantics document. This DTD is likely to become the standard for the description of object models in XML. Companies which produce documents which comply with standardized DTD's will be able to exploit any processing developed for use with those standardized DTD's."

[Concept Five Technologies, Inc., *Trident Next Generation Metadata Design and Generation Manual version 1.01*, pages 3-4, Copyright © 1998, 1999 by Hitachi, Ltd. and Concept Five Technologies, Inc.]

### 3.1.3 Domain Metadata

Interoperability requires convergence on data semantics description capabilities. The metadata in a BSA environment includes a description of the CORBA interfaces supported as well as the meta semantics related to specification of the analysis and input and output types supported by a particular analysis interface. The BSA metadata for the analysis type, inputs and outputs allows for the support of well understood multiple execution paths supported through the same simple interface.

The metadata provided by the valuetypes and XML is required to facilitate interoperability for analyses, inputs and outputs. Interoperability is achieved by providing run-time information about parameters required to perform an analysis. The client can dynamically interrogate the analysis service, learn about the input parameters, populate the input property set and perform the analysis. When the analysis is finished, the client can dynamically check the analysis service to learn about the output properties. The client can use this knowledge to dissect the outputs into information of interest.

The elements in the DsLSRAnalysis DTD correspond to the attributes in the previously defined **AnalysisType**, **InputPropertySpec**, and **OutputPropertySpec** value-types. In addition to the required valuetypes, the XML metadata may be available for the implementation to provide data about the analyses.

The attributes "type" used in the elements "input" and "output" contain a string represen-

tation of the **CORBA::TypeCode**. These representations conform to the following rules.

1. Basic IDL types are represented by a string containing the name of the type. The type is derived from the **CORBA TypeCode's TCKind** by deleting the leading "tk\_". This rule follows the convention used in section 5.3.10.2 (CorbaTypeName) of the XMI 1.0 specification (formal/00-06-01).

Example: the string representation of the type **long** is "ong;" that of **unsigned long long** is "ulonglong."

2. Sequences of basic IDL types are represented by a string containing the typespecifier in IDL syntax without any spaces. That is, a sequence of **XXXs** is coded as "sequence<XXX>" where XXX is the name of the string found using rule 1.

Example: A sequence of **longs** is represented by ""equence<long>."

3. For other data types, the repository ID is used.

Example: the **BioSequence** is represented by "IDL:omg.org/DsLSRBioObjects/BioSequence:1.1."

The elements have the same definition as the valuetype attributes previously specified. It is important to highlight the analysis type format. Again, the *type* element is used to specify both the correct classification of the analysis as well as a qualifier to specify category and additionally, provides information about the inputs to the analysis. The classification of the analysis could come from the BSA specified classification hierarchy as well as it could come from a hierarchy defined by a certain installation. A '/' is used to delimit the qualifier and a '.' is used to delimit the general input kind. An example of a specified *type* element would be *alignment.collection/assembly*.

The DTD has three places where vendor extension is available. The analysis, input and output elements specify an extension element that can be any valid content.

The following text presents the DTD for Biomolecular Sequence Analysis.

#### <!ELEMENT DsLSRAnalysis (analysis)+>

<!ELEMENT analysis (description?, input\*, output\*, analysis\_extension?)>

<!ATTLIST analysis

| CDATA #REQUIRED |
|-----------------|
| CDATA #IMPLIED  |
| CDATA #IMPLIED  |
| CDATA #IMPLIED  |
| CDATA #IMPLIED> |
|                 |

<!ELEMENT description ANY> <!ELEMENT extension ANY>

<!ELEMENT input (default?, allowed\*, input\_extension?)>

<!ATTLIST input

I

**CDATA #REQUIRED** type CDATA #REQUIRED name mandatory (true|false) "false"> <!ELEMENT default (#PCDATA)> <!ELEMENT allowed (#PCDATA)> <!ELEMENT output (output\_extension?)> <!ATTLIST output **CDATA #REQUIRED** type CDATA #REQUIRED> name <!ENTITY % vendor\_analysis\_tags "<!ELEMENT analysis\_extension EMPTY>"> <!ENTITY % vendor input tags "<!ELEMENT input extension EMPTY>"> <!ENTITY % vendor\_output\_tags "<!ELEMENT output\_extension EMPTY>"> %vendor\_analysis\_tags; %vendor input tags; %vendor\_output\_tags; The following text provides example XML that would be used with respect to the DsLSRAnalysis DTD. <?xml version="1.0" ?>

I

I

<!DOCTYPE DsLSRAnalysis SYSTEM "DsLSRAnalysis.dtd" >

<DsLSRAnalysis> <ANALYSIS TYPE = "search.list"> <INPUT NAME = "query\_sequence" TYPE = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0" MANDATORY = "true"> </INPUT> <INPUT NAME = "sequence\_list" TYPE = "IDL:omg.org/DsLSRBioObjects/BioSequenceList:1.0" MANDATORY = "true"> </INPUT> <OUTPUT NAME = "search\_result" TYPE = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0"> </OUTPUT> </ANALYSIS> </DsLSRAnalysis>

## 3.2 Classification of Analyses

This classification of analyses consists of three broad categories: searching, alignment, and utilities. Commonly used analyses are nicely partitioned into these categories.

### 3.2.1 Searching

Searching includes the broad category of similarity searching analyses. BLAST, FastA, and Smith-Waterman fall into this group. Searching can include querying **BioSequences** to identify **Annotations** that meet specified criteria. Searching also includes finding patterns and motifs in **BioSequences**. The results of these searches are **SeqRegions**. Examples include analyses such as PROSITE, BLOCKS, PRINTS, as well as most gene and ORF finding algorithms (e.g., GRAIL, GeneScan, GeneFind, and GLIMMER). It also includes identifying potential restriction enzyme and proteolytic cleavage sites.

The result of a search is a **SearchResult**. A **SearchResult** contains an array of **SearchHits**, which may be the specialized **SimilaritySearchHits**.

The searching hierarchy is:

- search (against a list, collection, or database)
- search/annotation
- search/region
- search/similarity (against a list, collection, or database)

#### 3.2.2 Alignment

The alignment category includes both pairwise and multiple alignments. No distinction is made. The result of either is an **Alignment**.

A sequence assembly contains both aligned sequences and unaligned sequences (fragments). The aligned sequences are represented by an **Alignment**. If one considers a phylogeny as an alignment of alignments, it too falls in this category.

The alignment hierarchy is:

- alignment (of a list or collection)
- alignment/assembly (of a list or collection)
- alignment/phylogeny

### 3.2.3 Utilities

There are several simple analyses that could either be viewed as analyses or simply provided as methods on an appropriately typed **BioSequence**. We decided to view them as simple analysis. This allowed us to keep the **BioSequence** interface simple. For example, simple sequence translation, using the standard genetic code, is provided by

NucleotideSequence's methods translate\_seq() and translate\_seq\_region(). A

3

more sophisticated sequence translation, allowing a user specified **GeneticCode**, is provided here.

The utilities category provides:

- utility/molecular\_weight
- utility/residue\_composition
- utility/ambiguous\_residues
- utility/gc\_content
- utility/isoelectric\_point
- utility/translate\_seq (uses GeneticCode)
- utility/translate\_seq\_region (uses GeneticCode)

# References

## A.1 List of References

I

Object Management Group. 1998. Biomolecular Sequence Analysis RFP. OMG Document lifesci/98-03-05.

Object Management Group. 1998. The Common Object Request Broker: Architecture and Specification, v2.2. OMG Document formal/98-07-01.

Object Management Group. 1998. CORBAservices: Common Object Services Specification. OMG Document formal/98-12-09.

Object Management Group. 1998. CORBAservices: Common Object Services IDL. OMG Document formal/98-10-53.

Object Management Group. 1998. CORBA v2.3a - Core final revision. OMG PC Document ptc/98-12-04.

Object Management Group. 1998. Interoperable Naming Service. OMG Document orbos/98-10-11.

Object Management Group. 1998. Joint Revised Objects by Value Submission - with Errata. OMG TC Document orbos/98-01-18.

Object Management Group. 1998. OMG IDL Style Guide. OMG Document ab/98-06-03.

Object Management Group. 2000. OMG XML Metadata Interchange (XMI) Specification. OMG Document formal/00-06-01.

Bairoch, Amos, et al. 1997. The Swiss-Prot Protein Sequence Data Bank User Manual. Release 35; November 1997.

Baldi, Pierre and Søren Brunak. 1998. Bioinformatics: The Machine Learning Approach. The MIT Press. ISBN: 0-262-02442-X.

Α

Baxevanis, Andreas D. and B.F. Francis Ouellette, eds. 1998. Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins. Wiley-Interscience. ISBN: 0-471-19196-5.

Elzanowski, Andrzej (Anjay) and Jim Ostell, compilers. 1996. The Genetic Codes. National Center for Biotechnology Information (NCBI). http://www.ncbi.nlm.nih.gov/htbin-post/Taxonomy/wprintgc?mode=t.

Gamma, Erich, Richard Helm, Ralph Johnson, and John Vlissides. 1995. Design Patterns: Elements of Reusable Object-Oriented Software. Addison-Wesley. ISBN: 0-201-63361-2.

Gusfield, Dan. 1997. Algorithms on Strings, Trees, and Sequences: Computer Science and Computational Biology. Cambridge Univ Pr (Short). ISBN: 0-521-58519-8.

IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for amino acids. http://www.chem.qmw.ac.uk/iupac/AminoAcid/.

IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) symbols for nucleic acids. http://www.chem.qmw.ac.uk/iubmb/misc/naseq.html.

IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) biostandards. http://www.chem.qmw.ac.uk/iubmb/nomenclature/.

Lander, Eric S., and Michael S. Waterman, eds. 1995. Calculating the Secrets of Life: Applications of the Mathematical Sciences in Molecular Biology. National Academy Press. ISBN: 0-309-04886-9.

National Center for Biotechnology Information, et al. 1997. The DDJB/EMBL/GenBank Feature Table: Definitions. Version 2.0. December 15, 1997.

Waterman, Michael S. 1995. Introduction to Computational Biology: Maps, Sequences, and Genomes. Chapman & Hall. ISBN: 0-412-99391-0.

# Genetic Codes

The genetic codes listed below were compiled by Andrzej (Anjay) Elzanowski and Jim Ostell (National Center for Biotechnology Information). See http://www.ncbi.nlm.nih.gov/htbin-post/Taxonomy/wprintgc?mode=t. "i" indicates initiation and alternative initiation codons.

## B.1 Standard

**B.2** Bacterial

TTT	F Phe	TCT S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC S Ser	TAC Y Tyr	TGC C Cys
TTA	L Leu	TCA S Ser	TAA * Ter	TGA * Ter
TTG	L Leu i	TCG S Ser	TAG * Ter	TGG W Trp
CTT	L Leu	CCT P Pro	CAT H His	CGT R Arg
CTC	L Leu	CCC P Pro	CAC H His	CGC R Arg
CTA	L Leu	CCA P Pro	CAA Q Gln	CGA R Arg
CTG	L Leu i	CCG P Pro	CAG Q Gln	CGG R Arg
ATT	I Ile	ACT T Thr	AAT N Asn	AGT S Ser
ATC	I Ile	ACC T Thr	AAC N Asn	AGC S Ser
ATA	I Ile	ACA T Thr	AAA K Lys	AGA R Arg
ATG	M Met i	ACG T Thr	AAG K Lys	AGG R Arg
GTT	V Val	GCT A Ala	GAT D Asp	GGT G Gly
GTC	V Val	GCC A Ala	GAC D Asp	GGC G Gly
GTA	V Val	GCA A Ala	GAA E Glu	GGA G Gly
GTG	V Val	GCG A Ala	GAG E Glu	GGG G Gly
TTT	F Phe	TCT S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC S Ser	TAC Y Tyr	TGC C Cys

Biomolecular Sequence Analysis Final Adopted Spec. November 2000


TTA	L Leu	TCA S	Ser	TAA	* Ter	TGA	* Ter
TTG	L Leu i	TCG S	Ser	TAG	* Ter	TGG	W Trp
CTT	L Leu	CCT P	Pro	CAT	H His	CGT	R Arg
CTC	L Leu	CCC P	Pro	CAC	H His	CGC	R Arg
CTA	L Leu	CCA P	Pro	CAA	Q Gln	CGA	R Arg
CTG	L Leu i	CCG P	Pro	CAG	Q Gln	CGG	R Arg
ATT	I Ile i	ACT T	Thr	AAT	N Asn	AGT	S Ser
ATC	I Ile i	ACC T	Thr	AAC	N Asn	AGC	S Ser
ATA	I Ile i	ACA T	Thr	AAA	K Lys	AGA	R Arg
ATG	M Met i	ACG T	Thr	AAG	K Lys	AGG	R Arg
GTT	V Val	GCT A	Ala	GAT	D Asp	GGT	G Gly
GTC	V Val	GCC A	Ala	GAC	D Asp	GGC	G Gly
GTA	V Val	GCA A	Ala	GAA	E Glu	GGA	G Gly
GTG	V Val i	GCG A	Ala	GAG	E Glu	GGG	G Gly

## B.3 Yeast Mitochondrial

	1			
TTT	F Phe	TCT S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC S Ser	TAC Y Tyr	TGC C Cys
TTA	L Leu	TCA S Ser	TAA * Ter	TGA W Trp
TTG	L Leu	TCG S Ser	TAG * Ter	TGG W Trp
CTT	T Thr	CCT P Pro	CAT H His	CGT R Arg
CTC	T Thr	CCC P Pro	CAC H His	CGC R Arg
CTA	T Thr	CCA P Pro	CAA Q Gln	CGA R Arg
CTG	T Thr	CCG P Pro	CAG Q Gln	CGG R Arg
ATT	I Ile	ACT T Thr	AAT N Asn	AGT S Ser
ATC	I Ile	ACC T Thr	AAC N Asn	AGC S Ser
ATA	M Met i	ACA T Thr	AAA K Lys	AGA R Arg
ATG	M Met i	ACG T Thr	AAG K Lys	AGG R Arg
GTT	V Val	GCT A Ala	GAT D Asp	GGT G Gly
GTC	V Val	GCC A Ala	GAC D Asp	GGC G Gly
GTA	V Val	GCA A Ala	GAA E Glu	GGA G Gly
GTG	V Val	GCG A Ala	GAG E Glu	GGG G Gly

# B.4 Vertebrate Mitochondrial

TTT	F Phe	TCT	S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC	S Ser	TAC Y Tyr	TGC C Cys
TTA	L Leu	TCA	S Ser	TAA * Ter	TGA W Trp
TTG	L Leu	TCG	S Ser	TAG * Ter	TGG W Trp
CTT	L Leu	CCT	P Pro	CAT H His	CGT R Arg
CTC	L Leu	CCC	P Pro	CAC H His	CGC R Arg

CTA CTG	L Leu L Leu	CCA P Pro CCG P Pro	CAA Q Gln CAG Q Gln	CGA R Arg CGG R Arg
010	2 200			
ATT	I Ile i	ACT T Thr	AAT N Asn	AGT S Ser
ATC	I Ile i	ACC T Thr	AAC N Asn	AGC S Ser
ATA	M Met i	ACA T Thr	AAA K Lys	AGA * Ter
ATG	M Met i	ACG T Thr	AAG K Lys	AGG * Ter
GTT	V Val	GCT A Ala	GAT D Asp	GGT G Gly
GTC	V Val	GCC A Ala	GAC D Asp	GGC G Gly
GTA	V Val	GCA A Ala	GAA E Glu	GGA G Gly
GTG	V Val i	GCG A Ala	GAG E Glu	GGG G Gly

## B.5 Mold Mitochondrial

TTT	F Phe	TCT S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC S Ser	TAC Y Tyr	TGC C Cys
TTA	L Leu i	TCA S Ser	TAA * Ter	TGA W Trp
TTG	L Leu i	TCG S Ser	TAG * Ter	TGG W Trp
CTT	L Leu	CCT P Pro	CAT H His	CGT R Arg
CTC	L Leu	CCC P Pro	CAC H His	CGC R Arg
CTA	L Leu	CCA P Pro	CAA Q Gln	CGA R Arg
CTG	L Leu i	CCG P Pro	CAG Q Gln	CGG R Arg
ATT	I Ile i	ACT T Thr	AAT N Asn	AGT S Ser
ATC	I Ile i	ACC T Thr	AAC N Asn	AGC S Ser
ATA	I Ile i	ACA T Thr	AAA K Lys	AGA R Arg
ATG	M Met i	ACG T Thr	AAG K Lys	AGG R Arg
GTT	V Val	GCT A Ala	GAT D Asp	GGT G Gly
GTC	V Val	GCC A Ala	GAC D Asp	GGC G Gly
GTA	V Val	GCA A Ala	GAA E Glu	GGA G Gly
GTG	V Val i	GCG A Ala	GAG E Glu	GGG G Gly

# B.6 Invertebrate Mitochondrial

TTT TTC	F Phe F Phe		S Ser S Ser		Y Tyr Y Tyr		C Cys C Cys
TTA	L Leu	TCA	S Ser	TAA '	* Ter	TGA	W Trp
TTG	L Leu i	TCG :	S Ser	TAG *	* Ter	TGG	W Trp
CTT	L Leu	CCT	P Pro	CAT F	H His	CGT	R Arg
CTC	L Leu	CCC 1	P Pro	CAC F	H His	CGC	R Arg
CTA	L Leu	CCA 1	P Pro	CAA Ç	Q Gln	CGA	R Arg
CTG	L Leu	CCG 1	P Pro	CAG Ç	Q Gln	CGG	R Arg
ATT	I Ile i	ACT :	T Thr	AAT N	N Asn	AGT	S Ser
ATC	I Ile i	ACC	T Thr	AAC N	N Asn	AGC	S Ser

ATA	M Met i	ACA T Tł	nr AAA	K Lys	AGA	S Ser
ATG	M Met i	ACG T Tł	nr AAG	K Lys	AGG	S Ser
GTT	V Val	GCT A A	la GAT	D Asp	GGT	G Gly
GTC	V Val	GCC A A	la GAC	D Asp	GGC	G Gly
GTA	V Val	GCA A A	la GAA	E Glu	GGA	G Gly
GTG	V Val i	GCG A Al	la GAG	E Glu	GGG	G Gly

## B.7 Echinoderm Mitochondrial

TTT	F Phe	TCT	S Ser	TAT	Y Tyr	TGT C Cys
TTC	F Phe	TCC	S Ser	TAC	Y Tyr	TGC C Cys
TTA	L Leu	TCA	S Ser	TAA	* Ter	TGA W Trp
TTG	L Leu	TCG	S Ser	TAG	* Ter	TGG W Trp
CTT	L Leu	CCT	P Pro	CAT	H His	CGT R Arg
CTC	L Leu	CCC	P Pro	CAC	H His	CGC R Arg
CTA	L Leu	CCA	P Pro	CAA	Q Gln	CGA R Arg
CTG	L Leu	CCG	P Pro	CAG	Q Gln	CGG R Arg
ATT	I Ile	ACT	T Thr	AAT	N Asn	AGT S Ser
ATC	I Ile	ACC	T Thr	AAC	N Asn	AGC S Ser
ATA	I Ile	ACA	T Thr	AAA	N Asn	AGA S Ser
ATG	M Met i	ACG	T Thr	AAG	K Lys	AGG S Ser
GTT	V Val	GCT	A Ala	GAT	D Asp	GGT G Gly
GTC	V Val	GCC	A Ala	GAC	D Asp	GGC G Gly
GTA	V Val	GCA	A Ala	GAA	E Glu	GGA G Gly
GTG	V Val	GCG	A Ala	GAG	E Glu	GGG G Gly

# B.8 Ascidian Mitochondrial

TTT	F Phe	TCT	S Ser	TAT	Y Tyr	TGT C Cys
		-		IAI	I IYI	
TTC	F Phe	TCC	S Ser	TAC	Y Tyr	TGC C Cys
TTA	L Leu	TCA	S Ser	TAA	* Ter	TGA W Trp
TTG	L Leu	TCG	S Ser	TAG	* Ter	TGG W Trp
CTT	L Leu	CCT	P Pro	CAT	H His	CGT R Arg
CTC	L Leu	CCC	P Pro	CAC	H His	CGC R Arg
CTA	L Leu	CCA	P Pro	CAA	Q Gln	CGA R Arg
CTG	L Leu	CCG	P Pro	CAG	Q Gln	CGG R Arg
ATT	I Ile	ACT	T Thr	AAT	N Asn	AGT S Ser
ATC	I Ile	ACC	T Thr	AAC	N Asn	AGC S Ser
ATA	M Met	ACA	T Thr	AAA	K Lys	AGA G Gly
ATG	M Met i	ACG	T Thr	AAG	K Lys	AGG G Gly
GTT	V Val	GCT	A Ala	GAT	D Asp	GGT G Gly
GTC	V Val	GCC	A Ala	GAC	D Asp	GGC G Gly

	GTA	v	Val	GCA	A	Ala	GAA	Е	Glu	GGA	G	Gly
	GTG	v	Val	GCG	Α	Ala	GAG	Е	Glu	GGG	G	Gly
B.9	Flatworm Mitochond	lria	al									
,												
	TTT	F	Phe	TCT	s	Ser	TAT	Y	Tyr	TGT	С	Cys
	TTC	F	Phe	TCC	s	Ser	TAC		- Tyr	TGC		Cys
	TTA	L	Leu	TCA	s	Ser	TAA	Y	Tyr	TGA		Trp
	TTG	L	Leu	TCG	S	Ser	TAG	*	Ter	TGG	W	Trp
	CTT	L	Leu	CCT	Р	Pro	CAT	н	His	CGT	R	Arg
	CTC	L	Leu	CCC	Р	Pro	CAC		His	CGC		Arg
	CTA	L	Leu	CCA	Ρ	Pro	CAA		Gln	CGA		Arg
	CTG	L	Leu	CCG	Ρ	Pro	CAG	Q	Gln	CGG	R	Arg
	3.000	-	TIA	2.00		The	220	NT	<b>1</b> am	200	~	
	ATT ATC		Ile Ile	ACT		Thr Thr	AAT		Asn	AGT		Ser
	ATA		Ile	ACC ACA		Thr	AAC AAA		Asn Asn	AGC AGA		Ser Ser
	ATG		Met i	ACG		Thr	AAG		Lys	AGG		Ser
	AIG	м	Met I	ACG	-	1111	ANG	ĸ	бүр	AGG	5	Der
	GTT	v	Val	GCT	A	Ala	GAT	D	Asp	GGT	G	Gly
	GTC	v	Val	GCC		Ala	GAC	D	Asp	GGC	G	Gly
	GTA	v	Val	GCA	А	Ala	GAA	Е	Glu	GGA	G	Gly
	GTG	v	Val	GCG	A	Ala	GAG	Е	Glu	GGG	G	Gly
R 10	Ciliate Nuclear											
<b>D</b> .10	Cillale Ivacieur											
	TTT	ਸ	Phe	TCT	S	Ser	TAT	v	Tyr	TGT	c	Cys
	TTC		Phe	TCC		Ser	TAC		Tyr	TGC		Cys
	TTA		Leu	TCA		Ser	TAA		Gln	TGA	*	Ter
	TTG		Leu	TCG		Ser	TAG		Gln	TGG		Trp
								~				
	CTT	L	Leu	CCT	Р	Pro	CAT	н	His	CGT	R	Arg
	CTC	L	Leu	CCC	Р	Pro	CAC	н	His	CGC	R	Arg
	CTA	L	Leu	CCA	Р	Pro	CAA	Q	Gln	CGA	R	Arg
	CTG	L	Leu	CCG	Ρ	Pro	CAG	Q	Gln	CGG	R	Arg
			_			_						
	ATT		Ile	ACT		Thr 	AAT		Asn	AGT		Ser
	ATC		Ile	ACC		Thr 	AAC		Asn	AGC		Ser
	ATA		Ile	ACA		Thr	AAA		Lys	AGA		Arg
	ATG	М	Met i	ACG	т	Thr	AAG	ĸ	Lys	AGG	R	Arg
	GTT	v	Val	GCT	Δ	Ala	GAT	п	Asp	GGT	G	Gly
	GII		Val			Ala	GAC		Asp	GGC		Gly
	GTA		Val	GCA		Ala	GAA		Glu	GGA		Gly
	GTG		Val	GCG		Ala	GAG		Glu	GGG		Gly
	515	•						-				1

# B.11 Euplotid Nuclear

TTT TTC	F Phe F Phe	TCT TCC	S Ser S Ser		Y Tyr Y Tyr	TGT C Cys TGC C Cys
-					-	-
TTA	L Leu	TCA	S Ser		* Ter	TGA C Cys
TTG	L Leu	TCG	S Ser	TAG	* Ter	TGG W Trp
CTT	L Leu	CCT	P Pro	CAT	H His	CGT R Arg
CTC	L Leu	CCC	P Pro	CAC	H His	CGC R Arg
CTA	L Leu	CCA	P Pro	CAA	Q Gln	CGA R Arg
CTG	L Leu	CCG	P Pro	CAG	Q Gln	CGG R Arg
ATT	I Ile	ACT	T Thr	AAT	N Asn	AGT S Ser
ATC	I Ile	ACC	T Thr	AAC	N Asn	AGC S Ser
ATA	I Ile	ACA	T Thr	AAA	K Lys	AGA R Arg
ATG	M Met i	ACG	T Thr	AAG	K Lys	AGG R Arg
GTT	V Val	GCT	A Ala	GAT	D Asp	GGT G Gly
GTC	V Val	GCC	A Ala	GAC	D Asp	GGC G Gly
GTA	V Val	GCA	A Ala	GAA	E Glu	GGA G Gly
GTG	V Val	GCG	A Ala	GAG	E Glu	GGG G Gly

## B.12 Alternative Yeast Nuclear

TTT	F Phe	TCT	S Ser	TAT	Y Tyr	TGT C Cys
TTC	F Phe	TCC	S Ser	TAC	Y Tyr	TGC C Cys
TTA	L Leu	TCA	S Ser	TAA	* Ter	TGA * Ter
TTG	L Leu	TCG	S Ser	TAG	* Ter	TGG W Trp
						-
CTT	L Leu	CCT	P Pro	CAT	H His	CGT R Arg
CTC	L Leu	CCC	P Pro	CAC	H His	CGC R Arg
CTA	L Leu	CCA	P Pro	CAA	Q Gln	CGA R Arg
CTG	S Ser i	CCG	P Pro	CAG	Q Gln	CGG R Arg
					~	<u> </u>
ATT	I Ile	ACT	T Thr	AAT	N Asn	AGT S Ser
ATC	I Ile	ACC	T Thr	AAC	N Asn	AGC S Ser
ATA	I Ile	ACA	T Thr	AAA	K Lys	AGA R Arg
		-			-	
ATG	M Met i	ACG	T Thr	AAG	K Lys	AGG R Arg
GTT	V Val	GCT	A Ala	GAT	D Asp	GGT G Gly
GTC	V Val	GCC	A Ala	GAC	D Asp	GGC G Gly
GTA	V Val	GCA	A Ala	GAA	E Glu	GGA G Gly
GTG	V Val	GCG	A Ala	GAG	E Glu	GGG G Gly
						-

# B.13 Blepharisma Macronuclear

TTT	F Phe	TCT	S Ser	TAT Y Tyr	TGT C Cys
TTC	F Phe	TCC	S Ser	TAC Y Tyr	TGC C Cys

TTA	L Leu	TCA S Ser	TAA * Ter	TGA * Ter
TTG	L Leu	TCG S Ser	TAG Q Gln	TGG W Trp
CTT	L Leu	CCT P Pro	CAT H His	CGT R Arg
CTC	L Leu	CCC P Pro	CAC H His	CGC R Arg
CTA	L Leu	CCA P Pro	CAA Q Gln	CGA R Arg
CTG	L Leu	CCG P Pro	CAG Q Gln	CGG R Arg
ATT	I Ile	ACT T Thr	AAT N Asn	AGT S Ser
ATC	I Ile	ACC T Thr	AAC N Asn	AGC S Ser
ATA	I Ile	ACA T Thr	AAA K Lys	AGA R Arg
ATG	M Met i	ACG T Thr	AAG K Lys	AGG R Arg
GTT	V Val	GCT A Ala	GAT D Asp	GGT G Gly
GTC	V Val	GCC A Ala	GAC D Asp	GGC G Gly
GTA	V Val	GCA A Ala	GAA E Glu	GGA G Gly
GTG	V Val	GCG A Ala	GAG E Glu	GGG G Gly

**B** 

## *Complete IDL*

### C.1 File: DsLSRBioObjects.idl

//File: DsLSRBioObjects.idl
// version: 29 October 2000.

#ifndef \_DS\_LSR\_BIOOBJECTS\_IDL\_ #define \_DS\_LSR\_BIOOBJECTS\_IDL\_

#pragma prefix "omg.org"

#include <CosLifeCycle.idl>
#include <CosPropertyService.idl>

module DsLSRBioObjects

typedef sequence<string> StringList; typedef string Identifier; typedef sequence<Identifier> IdentifierList;

enum StrandType {STRAND\_NOT\_KNOWN, STRAND\_NOT\_APPLICABLE, STRAND\_PLUS, STRAND\_MINUS, STRAND\_BOTH}; enum Basis {BASIS\_NOT\_KNOWN, BASIS\_NOT\_APPLICABLE, BASIS\_EXPERIMENTAL, BASIS\_COMPUTATIONAL, BASIS\_BOTH};

#pragma version Basis 1.1

valuetype Interval
{
 public unsigned long start;
 public unsigned long length;
}

};

{

I

I

```
valuetype SegRegion : Interval
   {
#pragma version SeqRegion 1.1
       public Identifier
                             id:
       public StrandType
                             strand type;
       public boolean
                              start relative to seq end;
   };
   typedef sequence<SeqRegion> SeqRegionList;
   valuetype CompositeSegRegion : SegRegion
   {
       enum SeqRegionOperator
       {
           NONE,
                          // Region has no sub regions or the sub regions
                          // don't need special treatment.
                          // Sub regions should be joined end-to-end to
           JOIN.
                          // form a contiguous region.
           ORDER
                          // Sub region order is important.
       };
       public SegRegionList
                                sub regions;
       public SeqRegionOperator region_operator;
   };
   interface Annotation : CosLifeCycle::LifeCycleObject
   {
       readonly attribute string
                                         name; // type of annotation
       readonly attribute any
                                         value; // the annotation
       readonly attribute Basis
                                         the_basis; // basis for annotation
       readonly attribute CosPropertyService::Properties qualifiers;
   };
   typedef sequence<Annotation> AnnotationList;
   exception IteratorInvalid
   {
       string reason;
   };
   interface AnnotationIterator
   {
       boolean
                    next(out Annotation the_annotation)
                          raises(IteratorInvalid);
       boolean
                    next_n(in unsigned long how_many,
                            out AnnotationList annotations)
                          raises(IteratorInvalid);
       void
                  reset();
       void
                  destroy();
   };
```

C-2

```
interface SeqAnnotation : Annotation
{
    readonly attribute SeqRegion seq_region;
};
typedef sequence<SeqAnnotation> SeqAnnotationList;
interface SeqAnnotationIterator
{
    boolean
                 next(out SeqAnnotation seq_annotation)
                      raises(IteratorInvalid);
    boolean
                 next_n(in unsigned long how_many,
                          out SeqAnnotationList seq_annotations)
                      raises(IteratorInvalid);
    void
               reset();
    void
               destroy();
};
exception IdentifierNotFound
{
    Identifier id;
};
exception IdentifierNotResolvable
{
    Identifier id:
    string reason;
};
exception IdentifierNotUnique
{
    Identifier id;
   IdentifierList ids;
};
exception IntervalOutOfBounds
{
    Interval invalid;
    Interval valid;
};
exception SeqRegionOutOfBounds
{
    SeqRegion invalid;
   Interval valid;
};
exception SeqRegionInvalid
{
    string reason;
```

I

I

I

}; exception NotUpdateable { string reason; }; interface BioSequence : CosLifeCycle::LifeCycleObject { **#pragma version BioSequence 1.1** readonly attribute string name; readonly attribute Identifier id: readonly attribute string description; readonly attribute string seq; readonly attribute unsigned long length; readonly attribute Basis the basis; string seq\_interval(in Interval the\_interval) raises(IntervalOutOfBounds, SeqRegionInvalid); get annotations( AnnotationList in unsigned long how\_many, in SeqRegion seq\_region, out AnnotationIterator the\_rest) raises(SeqRegionOutOfBounds, SeqRegionInvalid); num\_annotations(in SeqRegion seq\_region) unsigned long raises(SeqRegionOutOfBounds, SeqRegionInvalid); add annotation( void in Annotation the\_annotation) raises(NotUpdateable, SeqRegionOutOfBounds, SeqRegionInvalid); }; typedef sequence<BioSequence> BioSequenceList; typedef sequence<unsigned long> UnsignedLongList; exception ReadingFrameInvalid { short invalid; }; interface NucleotideSequence : BioSequence #pragma version NucleotideSequence 1.1 readonly attribute boolean circular; string reverse\_complement(); reverse\_complement\_interval(in Interval the\_interval) string

raises(IntervalOutOfBounds, SeqRegionInvalid);

I

	string string	translate_seq(
}	;	raises(SeqRegionOutOfBounds, SeqRegionInvalid);
t	ypedef seque	nce <nucleotidesequence> NucleotideSequenceList;</nucleotidesequence>
i {		noAcidSequence : BioSequence
#pra		AminoAcidSequence 1.1
t	ypedef seque	nce <aminoacidsequence> AminoAcidSequenceList;</aminoacidsequence>
	ypedef char ypedef char	
t	ypedef Base	Codon[3];
\ {	valuetype Cod [	eRule
}	public Coc public Res };	
t	typedef CodeF typedef string typedef seque	Rule Coding[64]; GeneticCodeName; nce <geneticcodename> GeneticCodeNameList;</geneticcodename>
e {	exception Inva	lidResidue
_	Residue th	ne_residue; ong offset;
i {	nterface Gene	ticCode
#pra	gma version (	GeneticCode 1.1
		ttribute Coding the_coding; ttribute GeneticCodeName name;
}		anslate_codon(in Codon the_codon) [InvalidResidue);

valuetype AlignmentElement

```
{
       public Object
                         element:
       public SeqRegion seq region;
       public string
                         key;
   };
   typedef sequence<AlignmentElement> AlignmentElementList;
   interface AlignmentElementIterator
   {
       boolean
                    next(out AlignmentElement element)
                     raises(IteratorInvalid);
       boolean
                    next_n(in unsigned long how_many,
                         out AlignmentElementList elements)
                     raises(IteratorInvalid);
       void
                  reset();
       void
                  destroy();
   };
   exception AlignmentObjectInvalid
   {
       Object element;
       string reason;
   };
   exception ElementNotInAlignment
   {
   };
   exception IndexOutOfBounds
   {
       unsigned long invalid;
       Interval valid;
   };
   interface Alignment : CosLifeCycle::LifeCycleObject
   {
#pragma version Alignment 1.1
       typedef string AlignType;
       typedef sequence<AlignType> AlignTypeList;
       const AlignType PROTEIN
                                           = "PROTEIN";
       const AlignType NON_PROTEIN
                                          = "NON_PROTEIN";
       const AlignType SEQUENCE_ERROR = "SEQUENCE_ERROR";
       const AlignType UNKNOWN
                                          = "UNKNOWN";
       AlignmentElementList get_alignment_elements(
              in unsigned long start,
              in unsigned long how_many,
              out AlignmentElementIterator the_rest)
```

```
raises(ElementNotInAlignment, IntervalOutOfBounds, SeqRegionInvalid);
raises(ElementNotInAlignment, IntervalOutOfBounds, SegRegionInvalid);
```

```
AlignType get align type by column(in unsigned long col)
   raises(IndexOutOfBounds);
```

```
};
```

```
typedef sequence<Alignment> AlignmentList;
```

raises(IndexOutOfBounds);

in Interval the interval)

in Interval the interval)

CompositeSeqRegion get gaps( in string key,

unsigned long num\_rows(); unsigned long num\_columns();

SeqRegion get\_seq\_region( in string key,

```
interface Assembly : Alignment
{
```

```
};
```

valuetype SearchHit

{ public Identifier id; public CosPropertyService::Properties hit\_info; };

typedef sequence<SearchHit> SearchHitList;

```
interface SearchHitlterator
```

```
{
                  next(out SearchHit hit)
    boolean
                   raises(IteratorInvalid);
    boolean
                  next_n(in unsigned long how_many,
                       out SearchHitList hit_list)
                   raises(IteratorInvalid);
    void
               reset();
    void
               destroy();
};
valuetype SimilaritySearchHit : SearchHit
{
    public AlignmentList alignment_list;
};
```

typedef sequence<SimilaritySearchHit> SimilaritySearchHitList;

```
interface BioSequenceIdentifierResolver
   {
       BioSequence resolve(in Identifier id)
           raises (IdentifierNotFound, IdentifierNotResolvable,
               IdentifierNotUnique);
   };
   interface SearchResult :
       BioSequenceldentifierResolver,
       CosLifeCycle::LifeCycleObject
   {
       readonly attribute BioSequence query sequence;
       readonly attribute CosPropertyService::Properties collection_info;
       StringList get property names();
       unsigned long num hits();
       SearchHitList get hits(
               in unsigned long start,
               in unsigned long how many,
               out SearchHitlterator the rest)
           raises (IndexOutOfBounds);
   };
   // optional interfaces
       interface AnnotationFactory
   {
#pragma version AnnotationFactory 1.1
       Annotation create_annotation(
               in string name,
               in any value,
               in Basis the_basis,
               in CosPropertyService::Properties qualifiers);
       SeqAnnotation create_seq_annotation(
               in string name,
               in any value,
               in Basis the_basis,
               in CosPropertyService::Properties qualifiers,
               in SeqRegion seq_region)
           raises (SeqRegionInvalid);
   };
   exception SeqAnnotationOutOfBounds
   {
       SeqAnnotation invalid;
       Interval valid;
   };
```

```
in Identifier id.
               in string description,
               in string residues,
               in Basis the basis,
               in boolean circular.
               in AnnotationList annotations)
           raises (InvalidResidue, SegAnnotationOutOfBounds, SegRegionInvalid);
   };
   interface AminoAcidSequenceFactory
   {
#pragma version AminoAcidSequenceFactory 1.1
       AminoAcidSequence create_sequence(
               in string name,
               in Identifier id.
               in string description,
               in string residues,
               in Basis the_basis,
               in AnnotationList annotations)
           raises (InvalidResidue, SeqAnnotationOutOfBounds, SeqRegionInvalid);
   };
   interface BioSequencelterator
   {
       boolean
                     next(out BioSequence seq)
                      raises(IteratorInvalid);
       boolean
                     next_n(in unsigned long how_many,
                          out BioSequenceList seqs)
                      raises(IteratorInvalid);
       void
                  reset():
       void
                  destroy();
   };
   interface NucleotideSequencelterator
   {
       boolean
                     next(out NucleotideSequence seq)
                      raises(IteratorInvalid);
                     next_n(in unsigned long how_many,
       boolean
                          out NucleotideSequenceList seqs)
                      raises(IteratorInvalid);
       void
                  reset();
       void
                  destroy();
```

interface NucleotideSequenceFactory

in string name,

#pragma version NucleotideSequenceFactory 1.1

NucleotideSequence create sequence(

{

```
};
```

```
interface AminoAcidSequenceIterator
{
   boolean
               next(out AminoAcidSequence seq)
                 raises(IteratorInvalid);
   boolean
               next n(in unsigned long how many,
                    out AminoAcidSequenceList seqs)
                 raises(IteratorInvalid);
   void
             reset();
   void
             destroy();
};
exception InvalidGeneticCodeName
{
   string invalid name;
};
interface GeneticCodeFactory
{
   const GeneticCodeName STANDARD
                                                          = "standard";
   const GeneticCodeName BACTERIAL
                                                          = "bacterial";
   const GeneticCodeName YEAST_MITOCHONDRIAL
                                                          = "yeast
       mitochondrial":
   const GeneticCodeName VERTEBRATE MITOCHONDRIAL = "vertebrate
       mitochondrial";
   const GeneticCodeName MOLD_MITOCHONDRIAL
                                                         = "mold
       mitochondrial";
   const GeneticCodeName INVERTEBRATE MITOCHONDRIAL= "invertebrate
       mitochondrial";
   const GeneticCodeName ECHINODERM_MITOCHONDRIAL= "echinoderm
       mitochondrial";
   const GeneticCodeName ASCIDIAN_MITOCHONDRIAL = "ascidian
       mitochondrial":
   const GeneticCodeName FLATWORM_MITOCHONDRIAL= "flatworm
       mitochondrial";
   const GeneticCodeName CILIATE_NUCLEAR
                                                      = "ciliate nuclear";
   const GeneticCodeName EUPLOTID_NUCLEAR
                                                      = "euplotid nuclear";
   const GeneticCodeName ALT_YEAST_NUCLEAR
                                                      = "alternative yeast
       nuclear":
   const GeneticCodeName BLEPHARISMA_MACRONUCLEAR = "blepharisma
       macronuclear";
   readonly attribute GeneticCodeNameList genetic_code_names;
   GeneticCode create_genetic_code(in GeneticCodeName name)
       raises(InvalidGeneticCodeName);
};
interface CharacterAlignmentEncoder
{
   readonly attribute Alignment the_alignment;
   unsigned long num_rows();
                                            // number of aligned
```

 $\boldsymbol{C}$ 

	unsigned l	long_num_columns();	// objects. Delegate // Delegate to Alignment
	string g	et_name(in unsigned long row) raises(IndexOutOfBounds);	// first object is in row // one etc
	StringList	get_all_names();	// all the Names
	string g	et_cell_contents(in unsigned long raises(IndexOutOfBounds);	row, in unsigned long col)
	boolean	<pre>is_cell_a_gap(in unsigned long ro raises(IndexOutOfBounds);</pre>	ow, in unsigned long col)
	unsigned l	long get_cell_width(in unsigned l raises(IndexOutOfBounds);	ong row, in unsigned long col)
	unsigned l	long max_column_width(in unsig raises(IndexOutOfBounds);	ned long col)
};	unsigned l	long max_width();	
int	erface Sing	leCharacterAlignmentEncoder : C	haracterAlignmentEncoder
{ #pragr	na version S	SingleCharacterAlignmentEncode	r 1.1
	string	get_row(in unsigned long row)	
	string	raises(IndexOutOfBounds); get_row_interval(in unsigned Ion raises(IndexOutOfBounds, In	
	StringList	SeqRegionInvalid); get_row_column_interval(in Inter raises(IntervalOutOfBounds,	
};	StringList		probably the most common!
	ception Can	notEncodeAlignment	
{	string reas	son;	
};			
int {	erface Char	acterAlignmentEncoderFactory	
ι		AlignmentEncoder create(in Align (CannotEncodeAlignment);	ment the_alignment)
};	Taises	(cannoteneodeAngninent),	
int {	erface Sing	leCharacterAlignmentEncoderFac	tory
·		racterAlignmentEncoder create(in (CannotEncodeAlignment);	Alignment the_alignment)
}; };			

#endif // \_DS\_LSR\_BIOOBJECTS\_IDL\_

I

### C.2 File: DsLSRAnalysis.idl

C

I

//File: DsLSRAnalysis.idl
// version: 29 October 2000.

#ifndef \_DS\_LSR\_ANALYSIS\_IDL\_
#define \_DS\_LSR\_ANALYSIS\_IDL\_

#pragma prefix "omg.org"

#include <orb.idl>
#include <CosPropertyService.idl>
#include <CosEventChannelAdmin.idl>
#include <CosLifeCycle.idl>
#include <TimeBase.idl>

module DsLSRAnalysis

typedef sequence<string> StringList;

valuetype AnalysisType

public string type; public string name; public string supplier; public string version; public string installation; public string description;

```
};
```

{

{

valuetype InputPropertySpec

```
{
```

public string name; public CORBA::TypeCode type; public boolean mandatory; public any default\_value; public any possible\_values; };

typedef sequence<InputPropertySpec> InputPropertySpecList;

valuetype OutputPropertySpec
{
 public string name;
 public CORBA::TypeCode type;
};

typedef sequence<OutputPropertySpec> OutputPropertySpecList;

enum AnalysisState

```
{
       CREATED, // Instance has been created but not yet executed.
       RUNNING, // The analysis instance is running.
       COMPLETED, // The instance has completed execution.
       TERMINATED BY REQUEST, // The instance was terminated by user request.
       TERMINATED BY ERROR // The instance terminated due to an error.
   };
   valuetype AnalysisEvent
   {
       public string message;
   };
   valuetype StateChangedEvent : truncatable AnalysisEvent
   {
#pragma version StateChangedEvent 1.1
       public AnalysisState previous state;
       public AnalysisState new_state;
   };
   valuetype HeartbeatProgressEvent : truncatable AnalysisEvent
   {
#pragma version HeartbeatProgressEvent 1.1
   };
   valuetype PercentProgressEvent : truncatable AnalysisEvent
#pragma version PercentProgressEvent 1.1
       public float percentage;
   }:
   valuetype TimeProgressEvent : truncatable AnalysisEvent
   {
#pragma version TimeProgressEvent 1.1
       public TimeBase::TimeT time_remaining;
   };
   valuetype StepProgressEvent : truncatable AnalysisEvent
#pragma version StepProgressEvent 1.1
       public unsigned long total_steps;
       public unsigned long steps_completed;
   };
```

interface AnalysisInstance;

typedef string MetaData;

I

C-13

```
exception DoesNotExistException { };
   interface AnalysisService
   {
       const string AnalysisTypeTag
                                        = "TAG ANALYSIS TYPE";
       const string InputPropertiesTag = "TAG INPUT PROPERTIES":
       const string OutputPropertiesTag = "TAG OUTPUT PROPERTIES";
       readonly attribute StringList metadata_tags;
       MetaData describe(in string tagname)
           raises (DoesNotExistException);
       readonly attribute AnalysisType type;
       readonly attribute InputPropertySpecList input_metadata;
       readonly attribute OutputPropertySpecList output_metadata;
       AnalysisInstance create analysis (in CosPropertyService::Properties input)
           raises (CosPropertyService::MultipleExceptions);
   };
   exception NotRunnable { };
   exception NotRunning { };
   exception NotTerminated
   {
       string reason;
   };
   interface JobControl
   {
#pragma version JobControl 1.1
       readonly attribute TimeBase::UtcT created;
       readonly attribute TimeBase::TimeT elapsed;
       readonly attribute TimeBase::UtcT started;
       readonly attribute TimeBase::UtcT ended;
       void run()
           raises (NotRunnable, CosPropertyService::MultipleExceptions);
       void terminate()
           raises (NotRunning, NotRunnable, NotTerminated);
       void wait()
           raises (NotRunning, NotRunnable);
   };
   interface AnalysisInstance : CosLifeCycle::LifeCycleObject
   {
       readonly attribute AnalysisService
                                            service:
       readonly attribute AnalysisState
                                            status;
       readonly attribute CosEventChannelAdmin::EventChannel event_channel;
       readonly attribute AnalysisEvent
                                           last_event;
```

I

```
readonly attribute JobControl job_control;
readonly attribute CosPropertyService::Properties inputs;
readonly attribute CosPropertyService::Properties results;
CosPropertyService::Properties get_result(in StringList name_list);
};
```

#endif // \_DS\_LSR\_ANALYSIS\_IDL\_

 $\boldsymbol{C}$ 

\_\_\_\_\_

# Domain Model DTD and XML

## D.1 File: DsLSRAnalysis.dtd

I

I

### <!ELEMENT DsLSRAnalysis (analysis)+>

<!ELEMENT analysis (description?, input\*, output\*, analysis\_extension?)>

<!ATTLIST analysis

| type         | CDATA #REQUIRED |
|--------------|-----------------|
| name         | CDATA #IMPLIED  |
| version      | CDATA #IMPLIED  |
| supplier     | CDATA #IMPLIED  |
| installation | CDATA #IMPLIED> |

<!ELEMENT description ANY>

<!ELEMENT input (default?, allowed\*, input\_extension?)>

<!ATTLIST input type CDATA #REQUIRED name CDATA #REQUIRED

mandatory (true|false) "false">

<!ELEMENT default (#PCDATA)> <!ELEMENT allowed (#PCDATA)>

<!ELEMENT output (output\_extension?)>

<!ATTLIST output

| type | CDATA #REQUIRED  |
|------|------------------|
| name | CDATA #REQUIRED> |

<!ENTITY % vendor\_analysis\_tags "<!ELEMENT analysis\_extension EMPTY>"> <!ENTITY % vendor\_input\_tags "<!ELEMENT input\_extension EMPTY>"> <!ENTITY % vendor\_output\_tags "<!ELEMENT output\_extension EMPTY>"> %vendor\_analysis\_tags; %vendor\_input\_tags; %vendor\_output\_tags;

### D.2 DsLSRBioAnalysis.xml

```
<?xml version = "1.0"?>
<!DOCTYPE DsLSRAnalysis SYSTEM "DsLSRAnalysis.dtd">
<DsLSRAnalysis>
   <analysis type = "search.list">
       <input
           name = "query_sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <input
           name = "sequence_list"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequenceList:1.0"
           mandatory = "true">
       </input>
       <output
           name = "search_result"
           type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
       </output>
   </analysis>
   <analysis type = "search.collection">
       <input
           name = "query_sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <input
           name = "sequence_iterator"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequenceIterator:1.0"
           mandatory = "true">
       </input>
       <output
           name = "search_result"
           type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
       </output>
   </analysis>
   <analysis type = "search.database">
       <input
           name = "query_sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <input
           name = "database_id"
           type = "IDL:omg.org/DsLSRBioObjects/Identifier:1.0"
```

```
mandatory = "true">
       </input>
       <output
           name = "search_result"
type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
       </output>
   </analysis>
   <analysis type = "search/annotation">
       <input
           name = "sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <output
           name = "sequence_annotation"
           type = "IDL:omg.org/DsLSRBioObjects/SeqAnnotationList:1.0">
       </output>
   </analysis>
   <analysis type = "search/region">
       <input
           name = "sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <output
           name = "sequence_region"
           type = "IDL:omg.org/DsLSRBioObjects/SeqRegionList:1.0">
       </output>
   </analysis>
   <analysis type = "search.list/similarity">
       <input
           name = "query_sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
       <input
           name = "sequence_list"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequenceList:1.0"
           mandatory = "true">
       </input>
       <output
           name = "search result"
           type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
       </output>
   </analysis>
   <analysis type = "search.collection/similarity">
       <input
           name = "query_sequence"
           type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
           mandatory = "true">
       </input>
```

```
<input
        name = "sequence_iterator"
        type = "IDL:omg.org/DsLSRBioObjects/BioSequenceIterator:1.0"
        mandatory = "true">
    </input>
    <output
        name = "search_result"
        type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
    </output>
</analysis>
<analysis type = "search.database/similarity">
    <input
        name = "query_sequence"
        type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
        mandatory = "true">
    </input>
    <input
       name = "database_id"
       type = "IDL:omg.org/DsLSRBioObjects/Identifier:1.0"
        mandatory = "true">
    </input>
    <output
        name = "search_result"
        type = "IDL:omg.org/DsLSRBioObjects/SearchResult:1.0">
    </output>
</analysis>
<analysis type = "alignment.list">
    <input
        name = "sequence_list"
       type = "IDL:omg.org/DsLSRBioObjects/BioSequenceList:1.0"
        mandatory = "true">
    </input>
    <output
        name = "alignment"
        type = "IDL:omg.org/DsLSRBioObjects/Alignment:1.0">
    </output>
</analysis>
<analysis type = "alignment.collection">
    <input
        name = "sequence_iterator"
       type = "IDL:omg.org/DsLSRBioObjects/BioSequenceIterator:1.0"
        mandatory = "true">
    </input>
    <output
        name = "alignment"
        type = "IDL:omg.org/DsLSRBioObjects/Alignment:1.0">
    </output>
</analysis>
<analysis type = "alignment.list/assembly">
    <input
       name = "sequence_list"
```

```
type = "IDL:omg.org/DsLSRBioObjects/BioSequenceList:1.0"
        mandatory = "true">
    </input>
    <output
        name = "assembly"
        type = "IDL:omg.org/DsLSRBioObjects/Assembly:1.0">
    </output>
</analysis>
<analysis type = "alignment.collection/assembly">
    <input
        name = "sequence_iterator"
       type = "IDL:omg.org/DsLSRBioObjects/BioSequenceIterator:1.0"
       mandatory = "true">
    </input>
    <output
       name = "assembly"
       type = "IDL:omg.org/DsLSRBioObjects/Assembly:1.0">
    </output>
</analysis>
<analysis type = "alignment/phylogeny">
    <input
        name = "alignment_list"
       type = "IDL:omg.org/DsLSRBioObjects/AlignmenList:1.0"
        mandatory = "true">
    </input>
    <output
        name = "alignment"
        type = "IDL:omg.org/DsLSRBioObjects/Alignment:1.0">
    </output>
</analysis>
<analysis type = "utility/molecular_weight">
    <input
        name = "sequence"
        type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
        mandatory = "true">
    </input>
    <output
       name = "molecular_weight"
       type = "unsigned long">
    </output>
</analysis>
<analysis type = "utility/residue_composition">
    <input
        name = "sequence"
        type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
        mandatory = "true">
    </input>
    <input
       name = "residue"
       type = "IDL:omg.org/DsLSRBioObjects/Residue:1.0"
        mandatory = "true">
```

```
</input>
    <output
        name = "residue_composition"
        type = "double">
    </output>
</analysis>
<analysis type = "utility/ambiguous_residues">
    <input
       name = "sequence"
       type = "IDL:omg.org/DsLSRBioObjects/BioSequence:1.0"
       mandatory = "true">
    </input>
    <input
        name = "genetic_code"
       type = "IDL:omg.org/DsLSRBioObjects/GeneticCode:1.0"
        mandatory = "true">
    </input>
    <output
       name = "ambiguous_residues"
       type = "boolean">
    </output>
</analysis>
<analysis type = "utility/gc_content">
    <input
        name = "sequence"
        type = "IDL:omg.org/DsLSRBioObjects/NucleicAcidSequence:1.0"
       mandatory = "true">
    </input>
    <output
       name = "gc_content"
       type = "double">
    </output>
</analysis>
<analysis type = "utility/isoelectric_point">
    <input
        name = "sequence"
       type = "IDL:omg.org/DsLSRBioObjects/AminoAcidSequence:1.0"
       mandatory = "true">
    </input>
    <output
       name = "isoelectric_point"
       type = "double">
    </output>
</analysis>
<analysis type = "utility/translate_seq">
    <input
       name = "sequence"
       type = "IDL:omg.org/DsLSRBioObjects/NucleicAcidSequence:1.0"
        mandatory = "true">
    </input>
    <input
```

```
name = "reading_frame"
       type = "short">
            <default>-3</default>
            <allowed>-2</allowed>
            <allowed>-1</allowed>
            <allowed>1</allowed>
            <allowed>2</allowed>
            <allowed>3</allowed>
    </input>
    <input
       name = "genetic_code"
       type = "IDL:omg.org/DsLSRBioObjects/GeneticCode:1.0"
       mandatory = "true">
    </input>
    <output
       name = "translated_seg"
       type = "string">
    </output>
</analysis>
<analysis type = "utility/translate_seq.seq_region">
   <input
       name = "sequence"
       type = "IDL:omg.org/DsLSRBioObjects/NucleicAcidSequence:1.0"
       mandatory = "true">
    </input>
    <input
       name = "sequence_region"
       type = "IDL:omg.org/DsLSRBioObjects/SeqRegion:1.0"
       mandatory = "true">
    </input>
    <input
       name = "genetic_code"
       type = "IDL:omg.org/DsLSRBioObjects/GeneticCode:1.0"
       mandatory = "true">
    </input>
    <output
       name = "translated_seg"
       type = "string">
    </output>
</analysis>
```

</DsLSRAnalysis>

D

# Future Direction of Metamodel

This specification uses metadata to describe analyses and inputs and outputs to analyses. Included in the specification is a DTD and example XML that shows the future direction of metadata within BSA. When more complex, more descriptive metadata is needed, the BSA metadata could be described using the mechanisms specified in the XMI. The sample better illustrates this idea.

### E.1 File: DsLSRAnalysis - future.dtd

<!-- LSR BSA DTD -->

<!ENTITY % UmlMetaData SYSTEM "ad98-10-16.dtd"> %UmlMetaData;

<!ENTITY % DsLSRAnalysisXMI SYSTEM "DsLSRAnalysisXMI.dtd"> %DsLSRAnalysisXMI;

### E.2 File: DsLSRAnalysisXMI - future.dtd

<!-- LSR BSA Analysis Machinery DTD -->

<!ELEMENT DsLSRAnalysisXMI (analysis)+> <!ATTLIST DsLSRAnalysisXMI %XMI.element.att; %XMI.link.att;

>

<!ELEMENT analysis (description?, input\*, output\*, XMI.extension\*)>

<!ATTLIST analysis

analysisType CDATA #REQUIRED name CDATA #IMPLIED version CDATA #IMPLIED

|   |  | supplier<br>installation   | CDATA #IMPLIED<br>CDATA #IMPLIED>                  |
|---|--|--|--|
|   | ELEMENT descriptio</th <th>n (XMI.extension*</th> <th>)&gt;</th>   | n (XMI.extension*  | )>   |
|   | ELEMENT input (para<br ATTLIST input</th <th colspan="2">:!ELEMENT input (parameter*, XMI.extension*)&gt;<br/>:!ATTLIST input</th>   | :!ELEMENT input (parameter*, XMI.extension*)><br>:!ATTLIST input |  |
|   |  | name<br>mandatory  | CDATA #REQUIRED<br>(true false) "false">           |
|   | ELEMENT output (pa<br ATTLIST output</th <th colspan="2"><!--ELEMENT output (parameter*, XMI.extension*)--></th>   | ELEMENT output (parameter*, XMI.extension*)                      |  |
|   |  | name   | CDATA #REQUIRED>                                   |
| ELEMENT parameter ((Foundation.Core.Parameter   logicalType), constraint*):</th <th>e.Parameter   logicalType), constraint*)&gt;</th> |  | e.Parameter   logicalType), constraint*)>                        |  |
|   | ELEMENT logicalType (Foundation.Core.DataType   XMI.CorbaTypeCode   XMI.extension+<br ELEMENT constraint (default?, allowed*, Foundation.Core.Constraint*, XMI.extension*) |  | re.DataType   XMI.CorbaTypeCode   XMI.extension+)> |
|   |  |  |  |
|   | ELEMENT default (#F</th <th>PCDATA)&gt;</th> <th></th>   | PCDATA)>   |  |
|   | ELEMENT allowed (#</th <th>PCDATA)&gt;</th> <th></th>  | PCDATA)>   |  |
| <i>E.3</i>  | E.3 File: DsLSRBioAnalysis - future (sample).xml<br>xml version="1.0" encoding="UTF-8"?<br>XMI SYSTEM 'DsLSRAnalysis-future.dtd'   |  |  |
|   |  |  |  |
|   | <xmi></xmi>  |  |  |
|   | <xmi.header><br/><xmi.model xmi.name<br=""><xmi.metamodel xmi.n<br=""></xmi.metamodel></xmi.model></xmi.header>  | •  |  |

<XMI.content/>

<XMI.extensions xmi.extender='omg.org/DsLSRAnalysis'>

### <DsLSRAnalysisXMI>

<analysis analysisType="similarity\_analysis/database">

<input name="query\_sequence" mandatory="true">

<parameter>

<Foundation.Core.Parameter> <Foundation.Core.ModelElement.name>input</Foundation.Core.ModelElement.name> <Foundation.Core.ModelElement.visibility xmi.value='public'/> <Foundation.Core.Parameter.defaultValue> <Foundation.Data\_Types.Expression/>

 $\boldsymbol{E}$ 

<Foundation.Core.Parameter.kind xmi.value='in'/>

<Foundation.Core.Parameter.type>

- <Foundation.Core.Interface>
- <Foundation.Core.ModelElement.name>BioSequence</Foundation.Core.Model Element.name>
- <Foundation.Core.ModelElement.visibility xmi.value='public'/>
- <Foundation.Core.GeneralizableElement.isRoot xmi.value='false'/>
- <Foundation.Core.GeneralizableElement.isLeaf xmi.value='false'/>
- <Foundation.Core.GeneralizableElement.isAbstract xmi.value='false'/>
- </Foundation.Core.Interface>
- </Foundation.Core.Parameter.type>
- </Foundation.Core.Parameter>

</parameter>

</input>

<input name="database\_id" mandatory="true">

#### <parameter>

- <Foundation.Core.Parameter> <Foundation.Core.ModelElement.name>input</Foundation.Core.ModelElement.name> <Foundation.Core.ModelElement.visibility xmi.value='public'/> <Foundation.Core.Parameter.defaultValue> <Foundation.Data\_Types.Expression/> </Foundation.Core.Parameter.defaultValue> <Foundation.Core.Parameter.kind xmi.value='in'/> <Foundation.Core.Parameter.type> <Foundation.Core.Interface> <Foundation.Core.ModelElement.name>Dbld</Foundation.Core.ModelElement.name> <Foundation.Core.ModelElement.visibility xmi.value='public'/> <Foundation.Core.GeneralizableElement.isRoot xmi.value='false'/> <Foundation.Core.GeneralizableElement.isLeaf xmi.value='false'/> <Foundation.Core.GeneralizableElement.isAbstract xmi.value='false'/></ Foundation.Core.Interface> </Foundation.Core.Parameter.type> </Foundation.Core.Parameter> <constraint> <allowed> database1 </allowed> <allowed> database2 </allowed> <allowed> database3 </allowed> <allowed> database4 </allowed>
- </constraint>

</parameter>

</input>

<output name="hits">

<parameter>

<Foundation.Core.Parameter> <Foundation.Core.ModelElement.name>input</Foundation.Core.ModelElement.name> <Foundation.Core.ModelElement.visibility xmi.value='public'/> <Foundation.Core.Parameter.defaultValue> <Foundation.Data\_Types.Expression/> </Foundation.Core.Parameter.defaultValue> <Foundation.Core.Parameter.kind xmi.value='out'/> <Foundation.Core.Parameter.type> <Foundation.Core.Interface> <Foundation.Core.ModelElement.name>Hits</Foundation.Core.ModelElement.name> <Foundation.Core.ModelElement.visibility xmi.value='public'/> <Foundation.Core.GeneralizableElement.isRoot xmi.value='false'/> <Foundation.Core.GeneralizableElement.isLeaf xmi.value='false'/> <Foundation.Core.GeneralizableElement.isAbstract xmi.value='false'/> </Foundation.Core.Interface> </Foundation.Core.Parameter.type> </Foundation.Core.Parameter>

</parameter>

</output>

</analysis>

</DsLSRAnalysisXMI>

</XMI.extensions> </XMI>

# Glossary

Glossary entries are organized alphabetically.

## Glossary Terms

Alignment	See Sequence Alignment
Ambiguity Code	Single character representation of an ambiguous nucleotide or residue.
Amino Acid	Any of a class of 20 small molecule building blocks that are combined to form proteins in living things (21 amino acids if selenocysteine is included). The sequence of amino acids in a protein and hence protein function are determined by the nucleotide sequence of its gene and the genetic code. The terms residue and amino acid are often used interchangeably.
Assembly	See Sequence Assembly
Base	See Nucleotide
Complementary Base	The nucleotide that chemically pairs up (hybridizes) with another nucleotide (called its complement) on the other strand, within a double-stranded sequence. G pairs with C in both DNA and RNA. A pairs with T in DNA. A pairs with U in RNA.
Complement	The sequence consisting of Complementary Bases.
Cladogram	See Phylogenetic Tree
Coding Sequence	A DNA sequence that contains appropriate start and stop codons, indicating the amino acid sequence translated from it could form a functional protein.
Codon	A set of three nucleotide bases in a DNA or RNA sequence, which together code for a unique amino acid. For example, the set AUG (adenine, uracil, guanine) codes for the amino acid methionine.

Contig or Contig Map	As used here, a graphical or data representation depicting the relative order of a linked library of small overlapping clones representing a complete chromosomal segment. See <i>Sequence Assembly</i> .
DNA (deoxyribonucleic acid)	The molecule that encodes genetic information. DNA is a double- stranded polymer of nucleotides. The two strands are held together by hydrogen bonds between base pairs of nucleotides. The four nucleotides in DNA contain the bases: adenine (A), guanine (G), cytosine (C), and thymine (T). In nature, base pairs form only between A and T and between G and C; thus the base sequence of each single strand can be deduced from that of its partner.
Expression	The conversion of the genetic instructions present in a DNA sequence into a unit of biological function in a living cell. Typically involves the process of transcription of a DNA sequence into an RNA sequence followed by translation of the RNA into protein. The RNA may be spliced before translation to remove introns.
Exon	Segment of a (genomic) sequence that is translated into a segment of a protein. See also <i>Intron</i> .
Gap	The opening and addition of one or more spaces to individual sequences in an alignment, in order to increase the consensus of the overall mapping. A gap represents a failure to establish equivalence between nucleotides in a particular region of a sequence when aligning it with one or more other sequences.
Gene	A length of DNA which codes for a particular protein, or in certain cases a functional or structural RNA molecule. Genes may be inferred from the DNA sequence by way of a coding sequence.
Genetic Code	The full set of codons in DNA or mRNA. Each codon is made up of three nucleotides which call for a unique amino acid. For example, the set AUG (adenine, uracil, guanine) calls for the amino acid methionine in the standard genetic code. The sequence of codons along an mRNA molecule specifies the sequence of amino acids in a particular protein.
Genome	The complete set of genetic information for a particular organism.
Genomic	Pertaining to or contained within a genome; also: chromosomal.
Hidden Markov Model (HMM)	A stochastic generative model for a series defined by a finite set of states, a discrete alphabet of symbols, a probability transition matrix, and a probability emission matrix.
Intron	Segment of the (genomic) sequence that is removed (spliced) from the RNA molecule prior to translation. Introns are therefore not translated to protein in a living cell.
Non-Coding	A class of genomic sequence that is not translated into a protein sequence. Non-coding sequence consists of introns and intergenic regions that may contain "junk" DNA such as repeat sequences.

Nucleic Acid	A polymer of nucleotides. DNA and RNA are different classes of nucleic acids. May be double- or single-stranded.
Nucleotide	A subunit of DNA or RNA consisting of a nitrogenous base (adenine, guanine, thymine, or cytosine in DNA; adenine, guanine, uracil, or cytosine in RNA), a phosphate molecule, and a sugar molecule (deoxyribose in DNA and ribose in RNA).
Phylogenetic Tree	A map, dendrogram, cladogram, or other data or graphical representation of a Phylogeny.
Phylogeny (phylogenesis, phylogenetic, phylogenic)	The evolutionary history of a particular taxonomic group, usually a species.
Profile	A table that lists the frequencies of finding each of the 20 amino acids at each position in conserved sequence pattern; used in sensitive sequence searches.
Protein	A biological molecule that consists of many amino acids chained together by peptide bonds. The sequence of amino acids in a protein is determined by the sequence of nucleotides in a DNA molecule. Proteins perform most of the enzymatic and structural roles within living cells.
RNA (ribonucleic acid)	A class of nucleic acids that consist of nucleotides containing the bases: adenine (A), guanine (G), cytosine (C), and uracil (U). An RNA molecule is typically single-stranded and can pair with DNA (where U pairs with A) or with another RNA molecule. RNA nucleotides are chemically distinct from DNA nucleotides and enable RNA molecules to have more complex structural and functional roles within a living cell.
Reading Frame	The 'phase' of the starting point of a translation. As each codon consists of three bases, a translation of a nucleotide sequence will yield entirely different protein sequences depending on this. Negative values are often used to denote translation of the reverse strand.
Residue	Amino acid; sometimes: nucleotide.
Reverse Complement	The sequence obtained by reading the opposite (complementary) strand of a nucleic acid sequence in the reverse direction.
Sequence	The order of nucleotides in a DNA or RNA molecule, or the order of amino acids in a protein.
Sequence Alignment	The explicit mapping between the residues of two or more sequences. A sequence alignment may have gaps. Alignments are used to establish similarities between sequences and/or sequence families.

Sequence Assembly	A series of linked sequence alignment analysis steps that is used for constructing a contig.
Splicing	The removal of introns from an RNA sequence leaving only the exons which are then translated into a protein.
Translation	The conversion of a nucleic acid sequence into an amino acid sequence according to the rules of a genetic code.