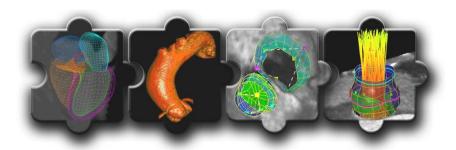
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Sim-e-Child Consortium

The partners in this project are:

- 01. Siemens AG (Siemens)
- 02. Lynkeus Srl (Lynkeus)
- 04. maat France (MAAT)
- 05. Technische Universität München (TUM)
- 06. I.R.C.C.S. Ospedale Pediatrico Bambino Gesù (OPBG)
- 07. Siemens Corporate Research, Inc. (SCR)
- 08. Johns Hopkins University (JHU)
- 10. American College of Cardiology Foundation (ACCF)
- 11. Siemens Program and System Engineering srl (PSE)

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List of contributors

Name	Affiliation	Co-author of
Razvan Ionasec	SCR	
Fabian Moerchen	SCR	
Jérôme Revillard	MAAT	
Kristóf Ralovich	TUM	

List of reviewers

Name	Affiliation
Michael Suehling	Siemens

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1. Introduction

The Sim-e-Child project proposes to develop a grid-enabled platform for large scale simulations in paediatric cardiology, providing a collaborative environment for constructing and validating multi-scale and personalized models of a growing heart and vessels. The objective of the Sim-e-Child is to strengthen the impact of the Health-e-Child project by creating an international simulation and validation environment for paediatric cardiology, supported by integrated data repositories. The project will advance the state-of-the-art by providing comprehensive and patient specific models for the dynamic and longitudinal interactions occurring in the left heart, with a focus on the congenital aortic arch disease and repair.

1.1. Purpose of the Document

The purpose of this document is to describe the high-level infrastructure along with the functional requirements of the Sim-e-Child platform. It identifies the major components, their functionalities, and interconnection with the Sim-e-Child platform. From a user perspective, this document provides an overview of the Sim-e-Child platform capabilities to perform simulations in a collaborative environment.

This is a revised version of the initial document D.2.1. Interoperability Requirements Specification, which includes updates regarding components and interfaces of the Sim-e-Child platform developed in the second project period.

1.2. Scope of the Document

This document defines the interoperability and functional requirements of the Sim-e-Child platform. The high-level architecture and brief description of the system components are initially introduced. Based on that, the platform functionalities are described by providing an overview of the use cases and simulation workflow. Interoperability is specified through the description of user and software interfaces. The document is concluded with the specification of the functional requirements.

With respect to the initial Interoperability Requirements Specification, this document includes the following updates:

- Revised component overview of the Sim-e-Child platform in Section 2.
- Extended simulation workflow overview to include aorta modelling in Section 2.2.
- Extended SimSys user interface to include aorta flow and anatomical measurements in Section 2.3.
- Revised specification of the software interface between SimSys and the GRID and SciPort components in Section 2.4.
- Extended requirements to support functionality for aorta modelling in Section 3.

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1.4. Abbreviations

CFD	Computational Fluid Dynamics
CT	Computed Tomography
DF	Desktop Fusion
DLL	Dynamic-link library
HeC	Health-e-Child
I/O	Input / Output
LA	Left Atrium
LV	Left Ventricle
MRI	Magnetic Resonance Imaging
MTOM	Message Transmission Optimization Mechanism
PC-MRI	Phase Contrast Magnetic Resonance Imaging
RV	Right Ventricle
SeC	Sim-e-Child
SOAP	Simple Object Access Protocol
UI	User Interface
WSDL	Web Service Description Language

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2. Overall Description

Sim-e-Child is a grid-enabled platform for large scale simulations in paediatric cardiology, providing a collaborative environment for constructing and validating multi-scale and personalized models of a growing heart and vessels.

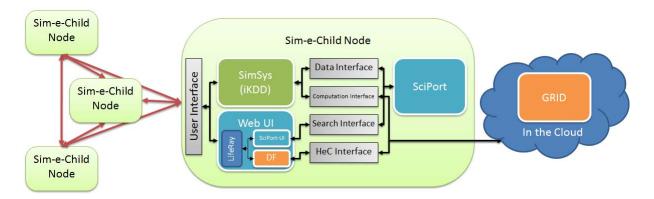


Figure 1: Sim-e-Child platform component overview

The Sim-e-Child is an extendable distributed platform that consists of Sim-e-Child Nodes running at different sites, which are interconnected through the Grid – SciPort network infrastructure (see Figure 1). Each Sim-e-Child Node is composed out of two core components: local SimSys client and WebUI (Web-Portal). In addition, a Grid Node may also include a local SciPort installation which is accessible locally and through the WebUI from anywhere. Each Sim-e-Child Node is connected to the GRID. The WebUI (Web-Portal) and Grid platform components are described in detail in the Deliverable D4.2, "Simulation and Collaboration Platform Interim Release and Report". Regardless of specific sites, users interact with the Sim-e-Child Platform through a unified User Interface, while the Sim-e-Child Node components communicate through three software interfaces: Data Interface, Computation Interface, Search Interface and HeC Interface.

The **SimSyS** provides workflows for patient-specific cardiac modelling and simulation of the left heart as well as advanced quantitative and qualitative analysis, and experiments validation capabilities.

The **WebUI** (http://sec-portal.maatg.fr/) integrates the Desktop Fusion system (remote desktop) which provides access to the Health-e-Child CaseReasoner. This later provides advanced browsing of the distributed case databases and selection of relevant cases from the Health-e-Child database. The unified Web-Portal also provides integrated access to the SciPort Web-UI for data search and management of the Sim-e-Child database. In addition, status information of submitted jobs can be monitored here.

The **SciPort** component handles the storage of all data available throughout the Sim-e-Child platform. Users can access data directly through the SciPort-UI or for further processing, modeling, simulation and advance visualization, through the SimSyS web service interface.

The **GRID** enables distributed resources for efficient computation of large scale simulation jobs. It accepts jobs submitted by the SimSys that can be monitored through the WebUI interface. The Grid is is available on regular servers that are always up and running. In

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addition, the platform capacity can be extended on demand by deploying more grid services inside cloud resources..

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2.1. Use Case Overview

The Sim-e-Child platform shall provide a variety of use cases that support clinicians to perform large-scale simulations and analysis of patient-specific cardiac models within an integrated and collaborative environment. The high-level use cases of Sim-e-Child are illustrated in Figure 2 and summarized in the reminder of this section.

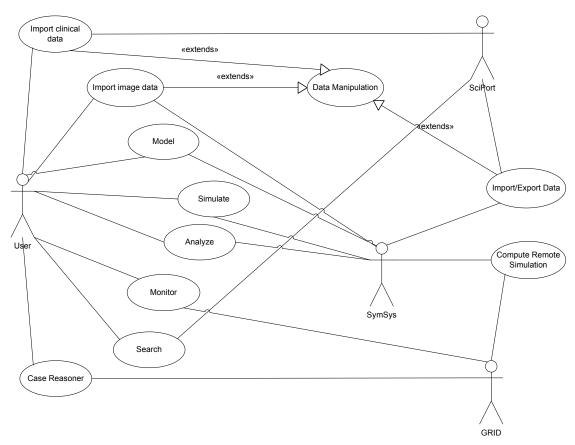


Figure 2: Sim-e-Child use case diagram

2.1.1. Data Manipulation

This use case encompasses the functionalities whereby data which is part of the Sim-e-Child platform and managed by SciPort is manipulated. In this case, data refers to imported images and clinical findings as well as information produced as a result of modelling, simulation or analysis activities. Core functionalities include the semi-automatic importing of image and clinical data, programmatic data transfer between SciPort and SimSys, and manual manipulation of existent entries.

2.1.2. Model

This use case captures functionalities related to the creation of patient-specific anatomical and dynamical models from imaging data, cardiac CT and cardiac MRI. Core modelling capabilities include the semi-automatic modelling of the LV, RV, Aortic Valve, Mitral Valve

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and Aorta from cardiac CT data, and LV, RV, Aorta, carotid arteries and blood-flow profiles from cardiac MRI data.

2.1.3. Simulate

This use case contains capabilities to perform CFD simulations from the patient-specific anatomical and dynamical models, and configurable boundary conditions. The use case also deals with capabilities to compute simulation jobs remotely on the GRID infrastructure.

2.1.4. Analyze

This use case comprises activities related to qualitative and quantitative analysis of data for a specific subject. It includes methods for measurement and visualization of anatomical, dynamical and hemodynamical information.

2.1.5. Monitor

This use case handles the monitoring of computation jobs executed remotely on the grid infrastructures. It enables progress monitoring as well as job prioritizing and cancellation.

2.1.6. Search

This use case contains capabilities to search the integrated patient records with clinical data, images, computational models and derived parameters. The user shall be able to search the integrated records combining different criteria on data fields and export the result as a spreadsheet with selected parameters or download selected cases including the image data and calculated models.

2.1.7. Case Reasoner

This use cases comprises functionalities related the Health-e-Child Case Reasoner that operate on the Health-e-Child data base.

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2.2. Simulation Workflow Overview

This section provides an overview of a common simulation workflow enabled by the Sim-e-Child platform. Figure 3 illustrates on the left side the activity diagram and on the right side the example outputs at four particular stages of the workflow.

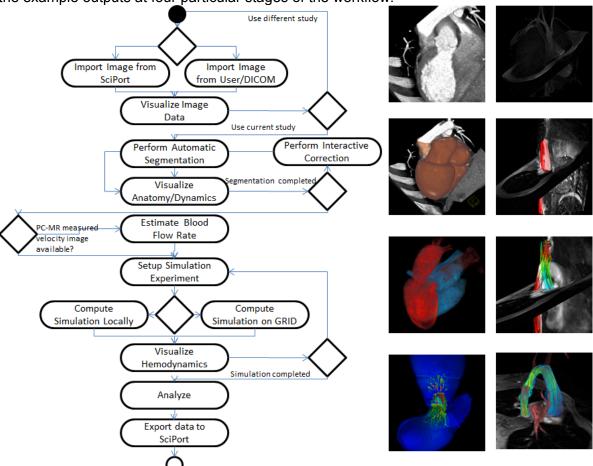


Figure 3: Sim-e-Child simulation workflow overview, Chambers and Aorta workflows

2.3. User Interfaces

The user interaction within the Sim-e-Child platform is handled through a common user interface, accessible at the location of deployment of each Sim-e-Child Node. Users have access to the local SimSys interface as well as to the Web User interface.

2.3.1. SimSys User Interface

The SimSys User Interface enables users to interact with the SimSys component and perform modeling, simulation and analysis of cardiac studies. This interface consists out of a workflow panel that guides users through a specific task and a rendering area, which interactively presents the current results of the processing using flow visualization, volume rendering, MPRs and graphs.

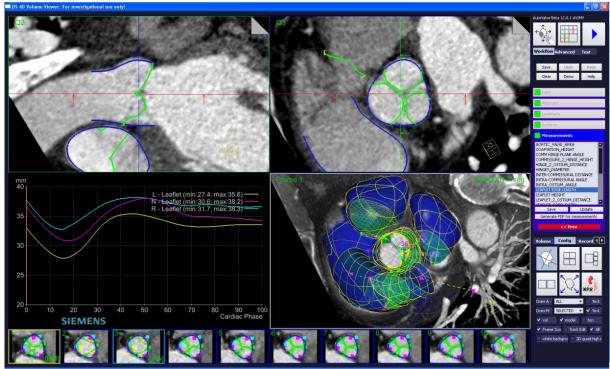


Figure 4: MPR views and volume rendering in SimSys during a Chambers and Valves workflow

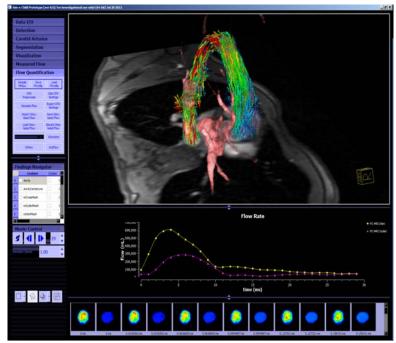


Figure 5: SimSys visualizing blood flow and showing flow analysis tools during an aorta workflow

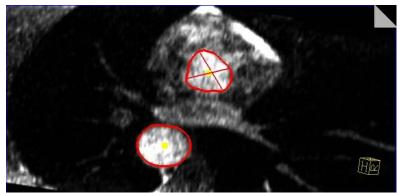
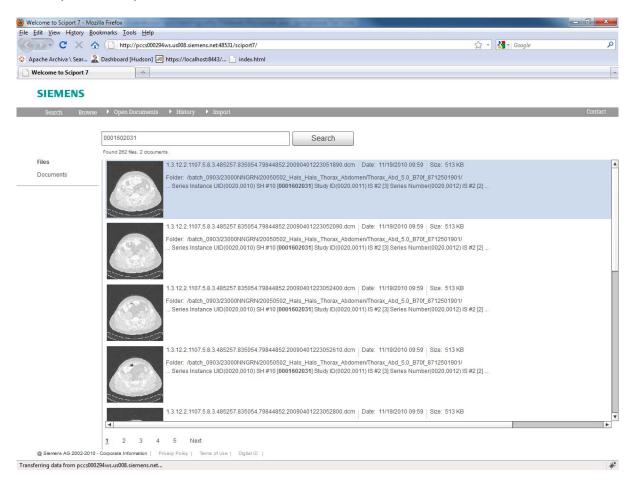


Figure 6: User interface of automated aorta lumen diameter measurements overlayed on a MR image.

2.3.2. SciPort Web Interface

The SciPort User Interface enables users to search the integrated electronic patient records by keyword and conditions of field from the clinical data and simulation parameters. In addition a folder-based structure can be browsed, the data can be modified via forms and forms can be customized. Data found through searching of browsing can be downloaded and exported as spreadsheets.



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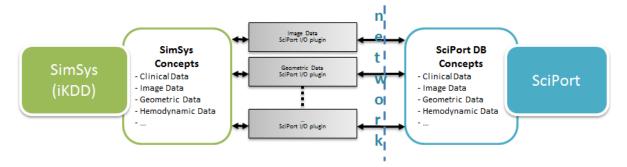
2.4. Software Interface

This section describes the three software interfaces that govern the communication between the Sim-e-Child components.

2.4.1. Data Interface

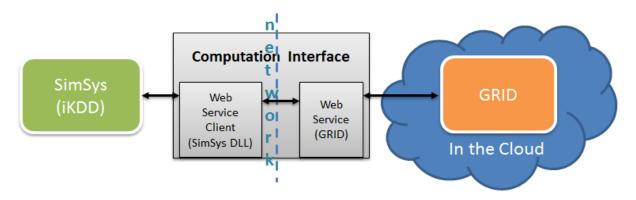
The following describes the interface between SimSys and the SciPort database components. Its core functionality enables for data stored into SciPort to be transparently loaded into SimSys concepts as well as transparent storing of SimSys concept into SciPort data objects. All data used within the SimSys is represented through a hierarchy of (SimSys) concepts. The data interface provides for each concept an I/O (input/output) module that serializes/deserializes SimSys concepts into SciPort concepts.

Through an IOServer, part of the SimSys, concepts can be loaded/stored from/to to SciPort provided the subject concept instance, database location (url and ID), and corresponding I/O plugin module that will perform the serialization/deserialization. The SciPort concepts are available to SimSys in forms of client libraries (plugin DLLs) that encapsulate the storage and retrieval from remote servers via secure web services.



2.4.2. Computation Interface

The following describes the interface between SimSys and GRID components. Its core functionality enables for computation tasks to be sent for execution on the GRID and for results to be returned to the SimSys. It also allows to send/receive parameters that control/monitor job execution. The connection of SimSys and GRID is realized through web services.



The computation interface is a web service. The client runs on the host machine of the Sime-Child node. The web service provider is deployed on the GRID. It is in charge of concretely executing and monitoring the jobs on the GRID middleware. As far as the monitoring part is concerned, it will implement push and pull notification mechanisms.

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As far as the web service client is concerned, it is implemented in form of a DLL plugin, which contains directly generated C++ stub code from the WSDL web service description. The DLL is linked and accessed directly, during runtime from the SimSys component. The monitoring notifications use a callback mechanism to notify the SimSys when new events/results are available.

Both the submission of a CFD simulation job and the retrieval of the simulation results to/from the GRID involves network transmission of large amounts of data (in the order of 100 MBs). To allow the sparse XML-based web service efficiently transferring such quantities, binary MTOM compression of simulation data is applied when embedding in the SOAP envelopes.

2.4.3. Search interface

The SciPort servers as part of the SeC nodes will support a transparent search via secure web services. The search interface of a SciPort server is abstracted via secure web service call. A client library knows of all the servers in the network. A search query is sent via secure webservice to all servers and the results are merged and returned to the client. This way the web interface served by each SeC node has access to the distributed database of integrated patient records.

2.4.4. HeC Interface

The HeC interface is a set of web services that are provided by the Pandora Gateway as described in the deliverable "D7.1 Health-e-Child Gateway Design Document and Developers' Guide".

It provides all the functionalities that are necessary to query the HeC databases and to do all the interactions that have to be done with the Grid middleware.

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3. Requirements

3.1. Requirements Modelling and Simulation

Sim-e-Child proposes a modular personalized cardiac modelling framework in which the left-ventricle, mitral valve, aortic valve, carotid arteries, and aorta will be modelled by taking into account the cross-dependency and joint function. The focus will be on the aortic arch disorders, i.e., aortic aneurysms and coarctation of the aorta, to provide morphological, dynamical and hemodynamical measures, simulations with predictive power, and virtual simulations of interventions.

(R1.1) Modelling of the Left Heart – segmentation capabilities of the aorta, LV, RV, and mitral and aortic valve from MRI data.

- Sim-e-Child shall integrate existing cardiac models from Health-e-Child and SCR (Zheng et al. 2007, Zheng et al. 2008, Ionasec et al. 2008, Ionasec et al. 2009).
- Patient-specific cardiac estimation from cardiac images shall be performed using robust discriminative learning methods, trained on large medical databases.
- Chambers workflow shall enable the semi-automatic patient-specific model estimation of the LV and RV from standard 3D/4D cardiac CT images and (cine) short-axis stacks of MRI images.
- Valve workflow shall enable the semi-automatic patient-specific model estimation of the aortic and mitral valves from standard 3D/4D cardiac CT images.
- Aorta workflow shall enable the semi-automatic patient-specific model estimation of the aorta from standard 3D/4D cardiac CT images and (cine) long-axis stacks of MRI images.

(R1.2) Flow Simulation – perform blood flow simulation using the CFD engine and capabilities to execute remotely.

- Sim-e-Child integrates the existent CFD solver from SCR to perform blood flow simulations (Mihalef et al. 2009, Mihalef et al. 2010).
- Aorta workflow enables the patient-specific hemodynamic simulation based on patient-specific dynamical models of the aorta and velocity inflow boundary conditions specified at the level of the aortic valve (Ralovich et al. 2011)
- Left-Heart workflow shall enable the patient-specific hemodynamic simulation based on patient-specific dynamical models of the LV, LA, aorta, aortic and mitral valves.
- For remote simulation execution input data and algorithm shall be incorporated in compressed binary objects

(R1.3) Advance Visualization and Analysis – Present capabilities for visualization the CFD results and perform advance quantitative and qualitative analysis

• Structural/Functional Analysis shall enable the measurement and visualization of clinical relevant parameters derived from patient-specific anatomical and dynamical models. During the aorta workflow SimSys provides the following automatic measurements: min/max aorta lumen diameter in arbitrary vessel cross sections (Figure 3), computation of flow rate based on PC-MR images, and simulated results.

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 Advanced Hemodynamical Analysis shall enable the computation, measurement and visualization of wall stress, wall shear stress, flow velocity, and flow vorticity from hemodynamic models. Vessel cross section analysis for local blood flow pattern assessment is included (Figure 3).

3.2. Requirements Storage and Collaboration

The SciPort (Wang et al. 2007) enables modelling of complex scientific information in a distributed environment with a web based user interface. A customized data model will be created in SciPort to store all information related to a Sim-e-Child heart simulations.

(R2.1) Data Manipulation – import, update, delete data using interactive manipulation, batch mode scripting or programmatic accessing.

- Allow design of complex SeC data model
- Import clinical data provided by physicians as relevant for the SeC modelling though batch process given spreadsheets with clinical parameters
- Import anonymized medical images provided by physicians through batch process given directory of files.
- Allow manual editing of patient data through web forms including deletion of records.
- Allow programmatic read/write access to patient records for simulation components to access image and clinical data and store simulation results.

(R2.2) Data Search - using meta-data, image attributes, image annotations and download of data of interest (distributed)

- Allow searching of integrated patient records combining conditions on clinical data, image attributes, model attributes and simulation results
- Allow searching across distributed interconnected SciPort servers
- Allow export of search results as spreadsheets and archives containing all images and models for a patient.

3.3. Requirements Computation

(R3.1) Remote Job Service – capabilities to submit a certain computation to be executed on the grid

- Allow to execute a job and to get the job unique identifier
- Allow to get the job results by providing the job unique identifier

(R3.2) Job Manager and Monitor – capabilities to manage / monitor and computation job currently running on the grid

- Allow to cancel a job by providing the job unique identifier
- Allow to get the job status by providing the job unique identifier

3.4. Health-e-Child Tools

(R4.1) HeC Case Reasoner access – The Sim-e-Child users that are authorised to do so must be able to use the Health-e-Child Case Reasoner through the LifeRay WebPortal. The Health-e-Child data must be accessible.