Virtual Organisation by Service Virtualisation: Conceptual Model and e-Science Application[1]

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Virtual organisation of collaborative networks frequently demands for information and communication technology to support coordination of cross-organisational business process chains. Service-oriented software technologies provide promising means to share software processes and services in collaborative networks but miss organisational abstractions and methodology. This paper proposes a conceptual model to mediate between organisational and technical levels. It introduces the concept of virtual business service to represent virtual organisations as service production networks and to support their coordination by means of service-oriented software technology. For illustration, we apply the proposed model to an e-Science scenario. We foster computational chemistry research by organisational virtualisation of a high-throughput computing laboratory. In particular, we model a polymorph prediction experiment as a virtual scientific service that facilitates planning and control of experimentation in a virtual research laboratory.

1. INTRODUCTION

After a period of process-orientation (Hammer and Champy 1993), current management research highlights the importance of networked organisations (Sydow 1992). In common strategic networks, participating companies gather their business processes into pools of core competencies. Subsequently, they loosely (re-)integrate these assets with respect to requirements of customers and markets. Figure 1.1 shows different co-operative constellations (N_i) of companies (M) relative to a strategic network (SN). Within the network, trust and information-integration between the participants allow restructuring value-chains whenever requirements change. In the extreme case of virtual organisation (VO) (Venkatraman and Henderson 1996), any organisational structure is just a virtual capability of the network. It is realised as a unique mission if and only if the respective business case occurs.

Yet, each strategic decision to (re-)structure the co-operative constellation within a network also affects the operational level. Establishing an operative business proc-

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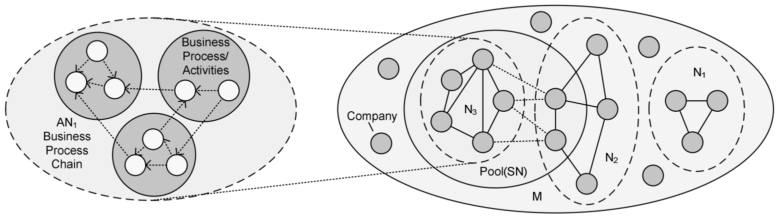

Figure 1.1 – Business process chains in networked organisations

ess chain for co-operation of participants requires regulation and enforcement of coordination. The strategy to coordinate participants and distribution of control between them relates to the requirements of a given mission. This essentially results in a specific interaction procedure between participants (see left hand side of fig.1.1).

The more dynamic the network, the more it relies on integration of information and communication technology (ICT) infrastructure between participants. Here, integration concerns two levels: the organisational information systems and the distributed middleware they build upon. In terms of middleware platforms, common specifications of Web Service and Grid Architectures (Alonso et al. 2004; Foster et al. 2002) provide effective means to share software services between participants of a strategic network. Respective middleware platforms provide notable technology support for secure, Internet-enabled software service interaction with shared data models and ontology. In terms of information system integration, cross-organizational workflow (e.g. CrossFlow (Grefen et al. 2000)) allows establishing business process chains between network participants by means of coordinating their software services. As a unifying paradigm, the emerging field of service-oriented computing (SOC) (Papazoglou and Georgakopoulos 2003) defines general abstractions of software service components and compositions together with development lifecycle methodology in accordance to business semantics, rules and processes.

However, current service-oriented software technologies do not fully address the requirements of collaborative networks. They demand for organisational models, engineering methodology and underlying middleware technology to create collaborative information systems that reflect the dynamic process chains of virtual organisations. Here, current technologies largely fail to deliver appropriate abstractions and lifecycle models for software development in sync with VO management. Common software service abstractions provide either too elemental or too specific abstractions for modelling VO process chains. Also, business process driven software service development lifecycle methodology is only just emerging (Papazoglou and van den Heuvel 2006) and rarely considers organisational context. Part of the problem is the lack of an appropriate conceptual model to mediate between the levels of VO and SOC. There is a clear need for a conceptual model that describes the particularities of VO and explains how its concepts effectively map to service-oriented software technologies.

In this paper, we propose a conceptual model of *virtual business services* for the abovementioned purpose. It builds on the assumption that the mission of a VO is to produce a commodity. This may include a physical product or not. It whatsoever always includes an intangible service as part or exclusively. Subsequently, we adopt an (economically) service based model of VO. We model collaborative business process chains as business service processes and VO as their providers. With this approach, we trace back essential tasks of regulating and enforcing VO coordination to planning and control of service production. Subsequently, service virtualisation allows supporting production planning and control by means of ICT mechanisms. In particular, patterns of virtual service processes map to common software service abstractions and allow utilising software service lifecycle methodology for planning and control of virtual business services.

The rest of the paper will describe and illustrate this approach. Section 2 proposes conceptual models for fundamental mechanics of business services and their virtualisation as well as management of virtual business service production networks. Section 3 extends the fundamental concepts into a reference model for pattern-based virtual business services. Section 4 introduces a scenario of computational chemistry e-Science that we use to evaluate our approach. Section 5 presents a case study that applies the reference model as a guide to model virtual organisation in the scenario. It outlines the design of polymorph prediction experiments as virtual scientific services and analyses the resulting properties of the respective virtual scientific laboratory. Section 6 deduces requirements for technologies to implement service virtualisation and assesses the utilisation of service-oriented software technology for that purpose. After a discussion of related work in section 7, the paper closes with a summary and outlook in section 8.

2. FUNDAMENTAL CONCEPTS OF VIRTUAL BUSINESS SERVICE PRODUCTION NETWORKS

The reference model we propose builds on a wider set of conceptual models including basic concepts of business services and production networks as well as their integrated virtualisation. This section will give a comprehensive introduction of the foundational models. It consecutively describes 1) models of business service transactions and processes, 2) models of strategic and virtual production networks and 3) a model of virtual production networks for business services.

Generally, conceptual modelling is about representing (part of) a complex situation in an abstract manner and with precise notation. Applications include the gathering and representation of information for the solution of complex problems from technical or organisational domains. Conceptual modelling often builds on object-oriented methods. They promote a good level of abstraction and potentially lead to comprehensive, maintainable and reusable models. Subsequently, we use the unified modelling language (UML), which seems appropriate for our rather abstract modelling level of VO concepts (Camarinha-Matos and Afsarmanesh 2006). UML offers common object-oriented abstractions as well as the ability to configure it for specification of application requirements and is therefore well suited for conceptual modelling. In particular, UML provides use case diagrams as means to model application domains. They show systems (in broader sense) on a high level of abstraction as use cases that are relevant to given actors. In the following, we utilise use case diagrams to specify our conceptual models.

2.1 Business Services (BS)

The first part of the conceptual models revolves around the notion of service. Figure 2.1 shows the conceptual model of *business services (BS)* as use case diagram that includes extension points for later use in subsequent models. It essentially adopts the three classical perspectives of economic service definition approaches: potential-, process- and result-orientation (Corsten 2001). We consider those as phases in a procedural model of service transactions that involves *client* and *provider* roles. Providers create potential for providing services in the *pre-contact phase*, while clients inspect and select them. Actual provision is happening in the *contact phase* that includes mutual activity and interaction of client and provider. Thereafter in the *post-contact phase*, providers offer support and are free to analyse and optimise their services. Clients do benefit from lasting effects of provision.

The crucial point why to look at services is the predominant characteristic of their contact phase essentially being an interaction process. Subsequently, we model the concept of *business service process (BSP)* as shown in figure 2.2.

The model refines the service contact phase as being composed of three types of

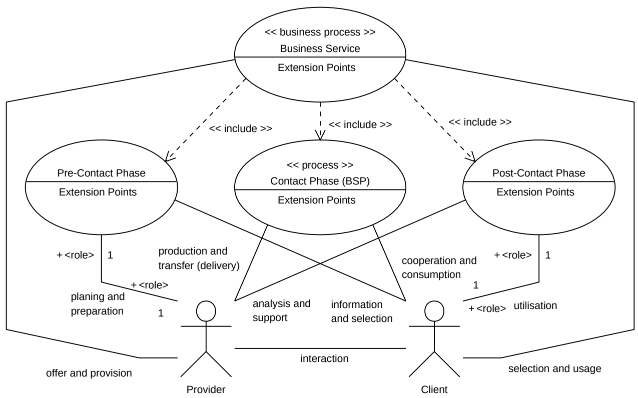

Figure 2.1 – Business Service (BS)

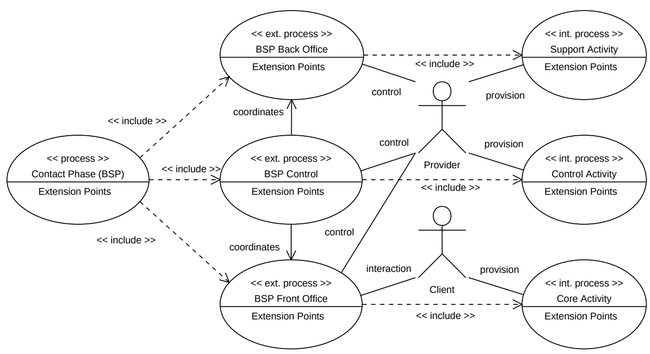

Figure 2.2 – Business Service Process (BSP)

processes. These represent classical concepts of service theory (Harms 2003): a *support process* or *back office* to involve and access local resources of the provider, a *control process* to coordinate the overall provision procedure and a *core process* or *front office* to interact with the client.

2.2 Virtual Production Networks (VPN)

The second part of the conceptual models captures concepts of network and virtual organisation. In particular, we perceive VO as a virtualised form of general *production network (PN)* (Eversheim, Schellberg, and Terhaag 2000). Production networks focus on the management aspects of collaborative networks that relate to co-operative production of some commodity. Figure 2.3 shows our model of production network concepts.

The conceptual model identifies the roles of *brokers*, *producers* and *coordinators*

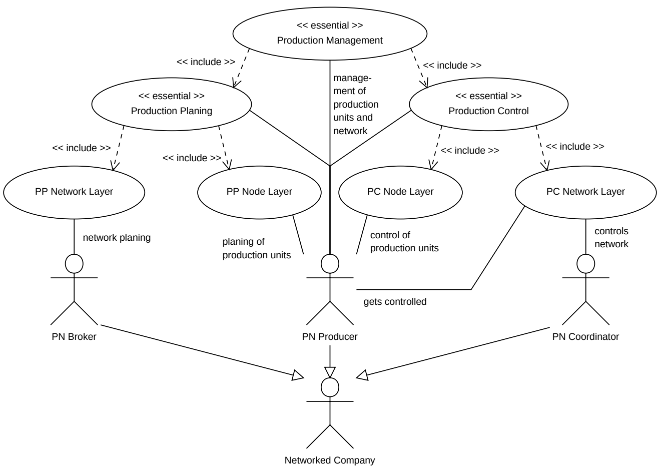

Figure 2.3 – Production Network (PN)

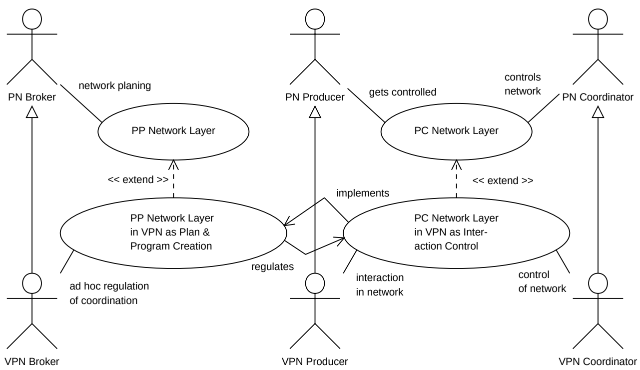

Figure 2.4 – Virtual Production Network (VPN)

as specialisations of general *networked companies*. *Production management* splits into *planning* and *control* on the level of *network* and *node*. We regard node-level management largely as self-contained responsibility of production units. The essential aspect is network-level management (of production), which includes regulation (planning) and enforcement (control) of coordination between co-operative activities of producers. Regulation and enforcement on network-level are responsibilities of broker and coordinator roles.

The subsequent model of *virtual production networks (VPN)* captures virtualisation of management aspects primarily on network-level. Figure 2.4 shows the model diagram. The crucial point is to be able to deal with regulation and enforcement of coordination in a frequent and ad hoc manner. Based on findings from organisation theory (Specht and Kahmann 2000), we assume that coordination is embodied in the complex interaction procedure between network participants. *VPN broker* utilise readily prepared programs and plans for their adaptation as means for ad hoc regulation. *VPN coordinators* enforce coordination rules by controlling the global interaction procedure of virtual production networks in operation.

2.3 Virtual Business Services Production Networks (VBSPN)

The conceptual base-models conclude with a combined model of service production in virtual production networks, where virtualisation of services allows for structuring and automating certain production management tasks. We refer to the resulting type of network as *virtual business service production network (VBSPN)*.

Figure 2.5 shows a model of derived roles in virtual service production networks. An initial observation identifies service clients as special producers of general service production networks, as they act as "external production factor" in service theory and actively participate in operational production of service processes. Members of a collaborative network in different roles take over the service provider part.

Virtualisation of an object refers to the substitution of its physical or institutional

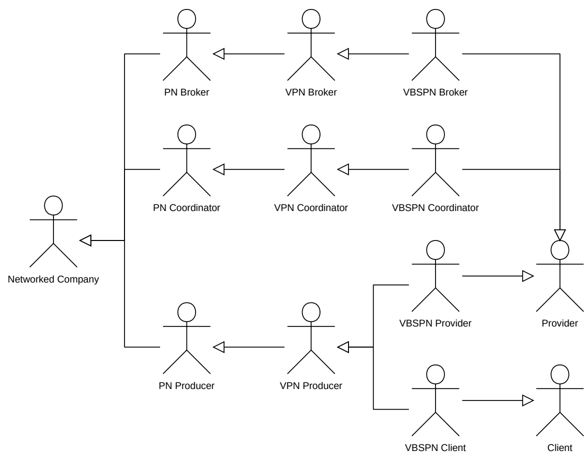

Figure 2.5 – Role Derivation for Virtual Business Service Production Networks

aspects with ICT representations, which leads to additional functionality or utility (Scholz 1996). It is the objective of our service virtualisation concept to replace the inherent service interaction procedure with an ICT-based interaction process, whereby this leads to the possibility of applying structured and automated methods to the VPN management tasks. Figure 2.6 shows the respective conceptual model of *virtual business services (VBS).*

The conceptual model of virtual business services is an extension of the conven-

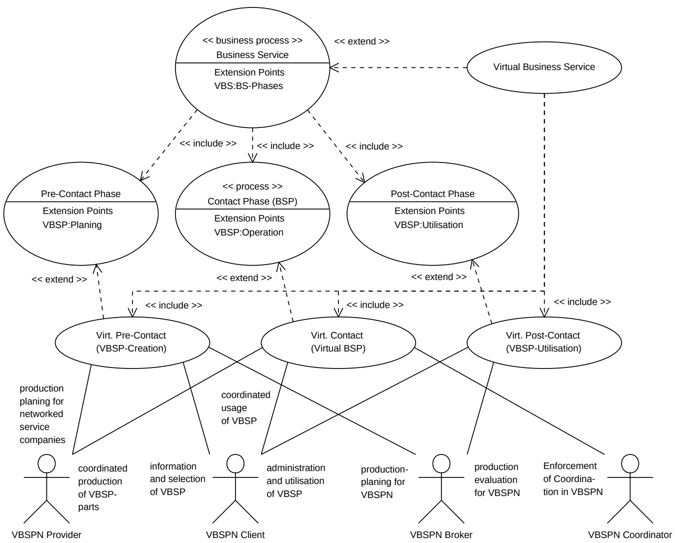

Figure 2.6 – Functions of VBSPN Actors

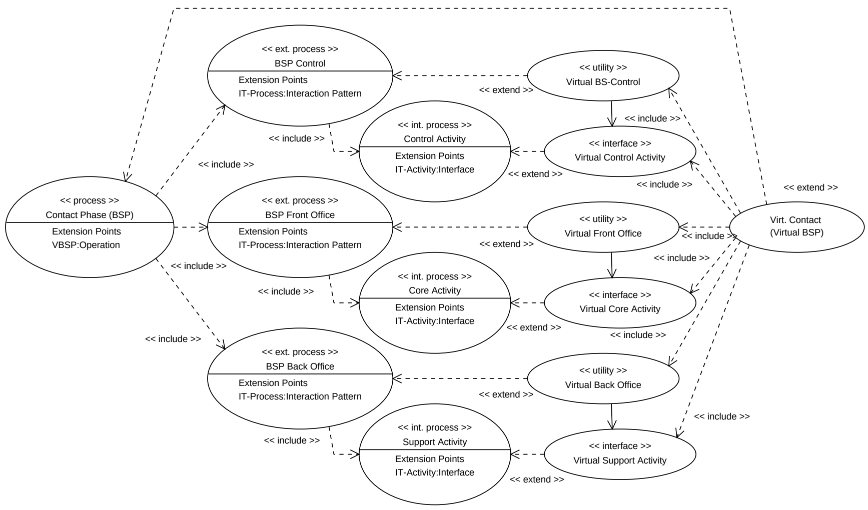

Figure 2.7 – Virtual Business Service Process (VBSP)

tional service phases by variations with respect to a *virtual business service process (VBSP).* This goes along with the mapping of role associations to the extended role model. Here, the associations of the service model roles with phases of service transactions merge with associations of VPN roles with the tasks of production management. The resulting responsibilities of roles are essentially enabled by the way in which virtualisation of the service process is achieved.

Figure 2.7 shows the virtualisation strategy for business service processes. It is twofold: On the one hand, we substitute service support, control and core processes by ICT representations of interaction process fragments. The latter allow for systematic development and automated execution. On the other hand, we assume that activities of network members that build on their internal processes provide communication endpoints for access on network-level. We substitute these endpoints by ICT-based interfaces that allow for exact specification and automated communication with external process parts.

Based on the service virtualisation strategy, we refine VPN management tasks into activities of the virtual service transaction and utilise substitution effects for their ICT support. Figure 2.8 models these associations.

The general idea is to perceive the interactive service process as embodiment of network coordination. Thus, operation of the virtual service process in the virtual

Figure 2.8 – VBSPN management

contact phase is a specialisation of network coordination enforcement. ICT representations of interaction process fragments and interfaces allow for formal specification and automated execution of network control. On the other side, planning and evaluation of the virtual service process in the virtual pre- and post-contact phases specialise network coordination regulation. Here, ICT representations of service process parts allow for their a priori development as programs and immediate enforcement by execution. Additionally, the definition of a structured development methodology allows planning for rapid adaptation of programs for individual virtual service production networks.

Altogether, the conceptual models show a strategy to utilise integrative ICT to plan and control coordinative rules for cooperative activities in collaborative networks. As we will show later, the grounding of the approach on top of generic service characteristics makes it particularly suitable for realisation by means of service-oriented software technologies.

3. A REFERENCE MODEL FOR VIRTUAL BUSINESS SERVICE PRODUCTION NETWORKS

After fundamental deduction of the general principles, we will now define an optimised reference model for VBSPNs. On the one hand, we will re-structure business service processes in order to streamline their virtualisation. On the other hand, we will introduce a pattern concept to support flexibility of business service processes for individual provision. The latter corresponds to the goal of supporting individual business process chains for the specific mission of a virtual organisation. We refer to this approach as *conceptual model of Pattern based Architectures for Service Interaction (PARIS).*

The basic idea behind the PARIS service model is to introduce and separate the concepts of *service content* and *provision*. Service content represents the actual business value of a service that constitutes its usefulness for clients. An example for this would be the presence and continuous maintenance of large data sets that stand behind an information service. Service provision refers to administrative procedures that make service content accessible to clients. Examples include authentication, metering or billing. With respect to this distinction, we refer to parts of the service process realising content as *service assets* and to those realising provision as *service capabilities*. Separation of service content and provision leads to some advantages as regards service virtualisation:

- *Content* corresponds to provider core competencies and *provision* to coordination of clients and providers. This mirrors the organisational structure of node- and network-level.
- *Content* often corresponds to physical processes. *Provision* often corresponds to informational processes. Respective structuring of sservice processes leads to partitions with homogeneous virtualisation potential. *Provision processes* often show a high potential of continuous virtualisation.

- Separation of *content* allows for its encapsulation and underpins the status of providers as autonomous companies.
- Separation of *provision* allows for integrative and joint virtualisation of interactive aspects of the service process for all involved roles.

In more detail, a service builds on a set of assets, jointly known as *service core*. Assets represent procedures that realise content. They are self-contained and encapsulate their details that remain internal to the producer. Their external interaction however is well defined and it is possible to combine assets without side effects. Each asset goes along with a capability that represents administrative procedures to access the content. We refer to such capabilities as *local capabilities*. In general, capabilities are self-contained and explicitly expose their details to any network participant. Their interaction procedures are well defined and they serve to coordinate involved roles. It is also possible to combine capabilities in order to assemble various assets into a service. Combination of local capabilities is subject to specific capabilities implementing global coordination. We refer to such capabilities as *global capabilities*. As the entire set of service capabilities literally wraps around service core assets, we refer to it as *service shell*.

3.1 Conceptual Service Model

Conceptual modelling of PARIS services builds on the fundamental models of virtual business service production networks up to the general model of virtual service transaction phases (figure 2.6). Subsequently, the PARIS virtual business service process is specialised as shown in figure 3.1. The major difference shows in an alternative process structure as regards separation of content and provision. The classical process structure, as introduced for business services, is present on the left. The three use cases in the middle of the diagram reflect the new structure. Here, *content* extends the case of support activity and leverages it to represent an internal process of a provider. A symmetrical case exists for core activity as an internal process of a client that we refer to as *demand*. Control activities together with all external parts of the service process merge into a single case *provision* that represents interaction processes to coordinate administrative procedures between clients and providers.

Similar to the fundamental models, we then extend the cases of the alternative service process into virtualised counterparts. We extend content and demand into *assets* and *consumption*. As explained above, extension leverages the interaction aspect and introduces virtualisation by substitutions in the form of ICT-based interfaces. We further extend provision into *capabilities* with *local* and *global* refinements. Again, extension leverages the interaction aspect and introduces virtualisation by substitutions in form of ICT-based interaction processes. Together, assets, demands and capabilities make up the *PARIS virtual business service process*. Compared to the fundamental model it shows a more pragmatic set of concepts that consider characteristics of organisational structure and virtualisation.

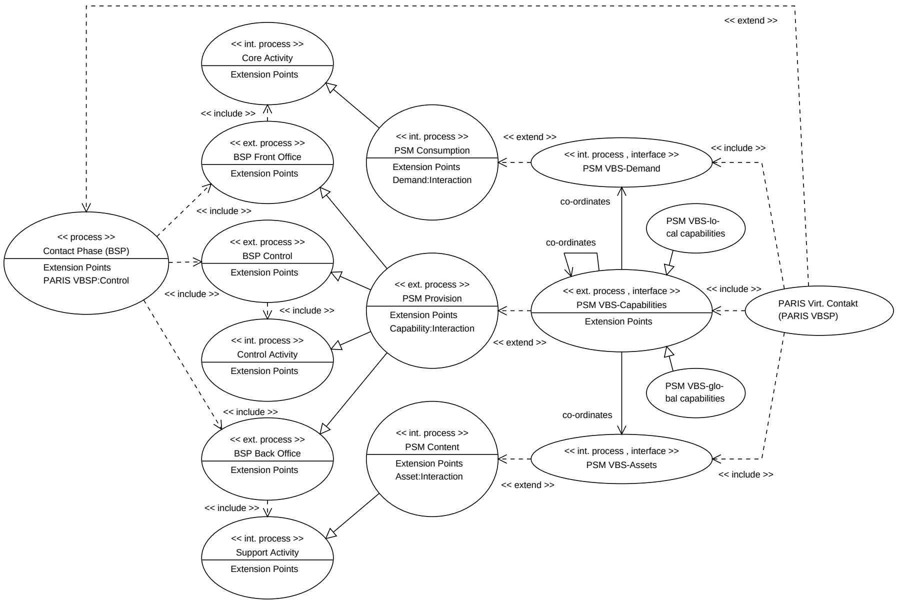

Figure 3.1 – Interaction Centred Structuring of Virtual Service Process

3.2 Virtual Service Production Control

Based on the concepts of PARIS virtual service processes, figure 3.2 shows a diagram that models respective responsibilities of roles related to virtual service production *control*. Roles essentially refine those of the fundamental conceptual models. In terms of control however, the coordinator role splits into distinct responsibilities of network producers and broker. Producers are obliged to control local capabilities related to their assets. In turn, the network broker takes over control of global capabilities that embody coordination of the service as a whole. Together, local and global service capabilities build a specialised form of production control that enforces coordinative regulations on network-level. Furthermore, we anticipate the operational variation of capabilities with respect to specific missions of service provision. We address this by the case of specific *enforcement.* Enforcements are variable instances of general coordinative regulations that cater for specific requirements of a mission. As we will show in our case study, such variation of enforcement especially affects non-functional properties of business services.

Like in the fundamental model, service production control on node-level comes in a specialised form of virtualised support and control activities. These are present as assets and demands in the PARIS virtual service process model. Producer and client roles take over responsibility for implementation and control of these management cases that relate to their internal processes.

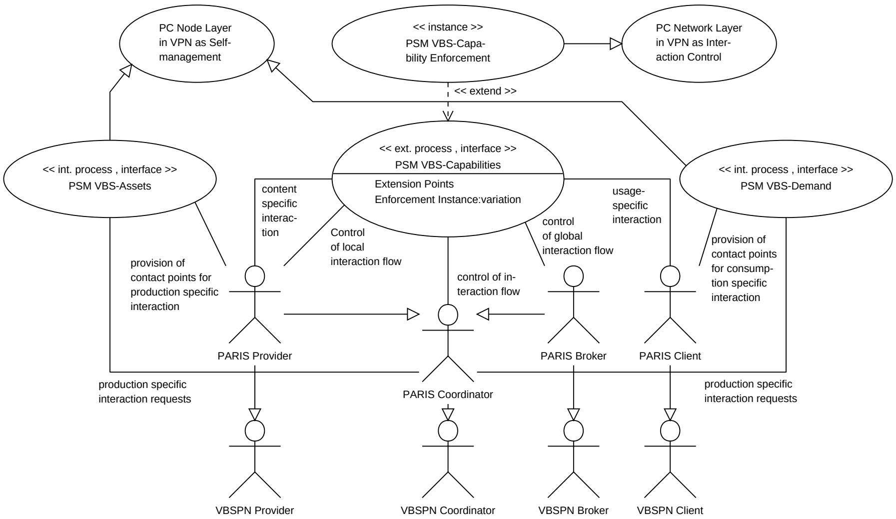

Figure 3.2 – Control-Related Role Functions and Variation Points

3.3 Virtual Service Production Planning

The last part of the reference model concerns virtual service production *planning.* Figure 3.3 shows the respective model. It builds on an extended perspective of the fundamental model (upper part of figure 2.8). The extended perspective additionally covers use cases that make up creation and utilisation of virtual business service processes (VBSP) on network- and node-level.

On node-level, providers are concerned with VBSP creation in two cases. First, they plan and create support activities they are intending to provide. Second, they adjust them with respect to the global service process. In the PARIS model, providers do not only develop internal assets, but also related local capabilities. They adjust their local capabilities with respect to global capabilities, thereby focusing on interaction. Clients are involved in VBSP creation by adjusting their demands with the offered service process. In terms of VBSP utilisation, they are evaluating the experience of a VBSP instance. We note that the scope of adjustment and evaluation tasks is explicitly restricted to the interaction aspect that becomes visible in form of capabilities.

On network-level of the fundamental model, VBSP creation involves a broker that plans and creates control aspects of VBSP and adjusts them with respect to support and core activities. As regards VBSP utilisation, brokers evaluate VBSP instances in terms of effectiveness and efficiency. The PARIS model extends the fundamental cases. Here, brokers are sighting asset-specific local capabilities of providers and developing coordinative global capabilities to integrate them into a complete virtual business service process. After provision of a service, they analyse the actual interactions that resulted from the control process of capability enforcement.

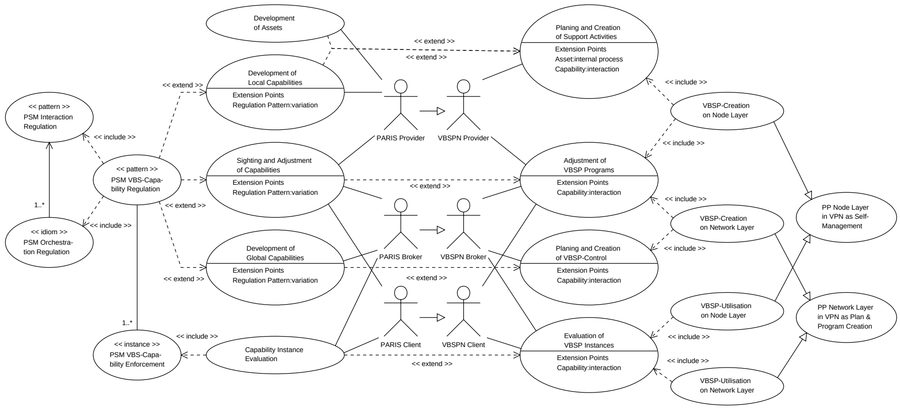

Figure 3.3 – Planning-Related Role Functions and Variation Points

Planning variations of VBSPs

As regards support of individual service processes, we propose pattern-based extensions of planning and control use cases. In terms of virtual service production planning, we extend PARIS use cases related to the development of capabilities into a regulation activity that utilises patterns of coordination. In terms of virtual service production control, we extend PARIS use cases of capabilities within the virtual service process into an enforcement activity that is one of many possible instances of a coordination pattern.

The crucial feature of this concept is the 1-n relationship of pattern regulation and instance enforcement cases. Pattern-based regulation covers a) general principles to coordinate providers and clients as well as b) various specific possibilities to enforce them. With respect to the underlying concept of interaction-based service process virtualisation, we capture general principles of coordination as design patterns of interaction flow (interaction patterns) and refer to this type of planning as *interaction regulation*. Subsequently, we capture variations of coordination enforcement as implementation patterns of interaction flow orchestration (orchestration idioms) and refer to their planning as *orchestration regulation*.

The application of each of the various orchestration idioms to the interaction pattern leads to resolution of the regulative patterns into a distinct enforcing instance. Such an instance is effectively an operational interaction control procedure with individual non-functional properties. Based on those properties, resolution of regulative patterns into enforcing instances happens ad hoc with respect to requirements of a specific mission.

4. SCENARIO: VIRTUAL ORGANISATION IN E-SCIENCE

We will now introduce a scenario of single organisation production that promises particular high potential for as well as benefit from virtual organisation. The scenario comes from the context of e-Science in the field of computational chemistry. It builds on the research method of polymorph prediction and its implementation in computational grids. Next, we will first outline the research method in general. Then we describe its grid-based implementation at University College London (UCL) and its extension to a virtual laboratory in the UK e-Science network. In particular, we will highlight requirements of experimental variation.

4.1 Polymorph Prediction Research Method

The research method of polymorph prediction builds on the observation that organic molecules tend to appear in different forms of crystal structures (polymorphs) that exhibit distinct physical properties. For many molecules, the range of polymorphs is initially unknown. Utilisation of molecules however depends on their physical properties and prediction of their polymorphs is therefore highly desirable (e.g. in pharmaceutical industry, patents need to refer to specific polymorphs).

The computational approach to polymorph prediction tackles the problem in a systematic way (Price 2004). The idea is to first compute (parts of) the theoretical packing of a molecule into crystal structures with algorithms like MOLPAK (Holden, Du, and Ammon 1993). The next step is to compute the physical properties of each crystal structure (to a certain degree of accuracy) with algorithms like DMAREL (Willock et al. 1995). Finally, scientists assess lattice energy and molecular volume of different crystal structures to predict their thermodynamic plausibility.

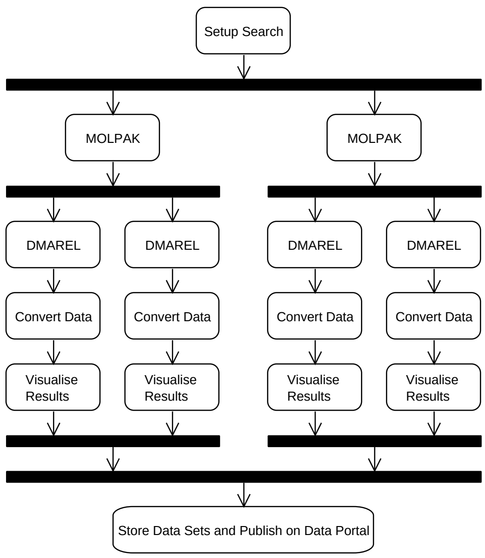

Figure 4.1 – Polymorphic Search Workflow (Emmerich et al. 2005)

Figure 4.1 shows the process of computational polymorph prediction experiments. It starts with specification of the molecule in question as well as search parameters like the range of packing and required accuracy of properties. The following computations are generally independent and therefore split into parallel runs of MOLPAK and DMAREL algorithms. In the end (and actually in between), result data needs to be converted into formats acceptable by algorithms to compute and human scientists to access. The later case takes the form of visualisation into scatter plot diagrams. Finally, result data is persisted into a database and possibly published for access by collaborating scientists.

4.2 Organisation and Virtualisation of Polymorph Prediction Laboratories

Due to its high computational demand and natural parallelism, the computational approach to polymorph prediction can considerably benefit from grid-based implementation in general and high throughput computing in particular (Nowell et al. 2004). An according implementation of polymorph search processes has been realised at University College London (Emmerich et al. 2005). It uses workflow-based software service compositions to capture the experiment process and control execution of its activities in different organisational units. Those units are thereby effectively integrated into an e-Science laboratory for polymorph prediction.

At the moment, the laboratory mainly consists of an interactive workplace and result database at the UCL chemistry department, experimental control and other auxiliary functions (e.g. data transformation) at the UCL computer science department and the UCL Condor high-throughput commodity computing pool for experiment computations.

As it turned out, even the very large Condor pool at UCL (980+ nodes) is fully utilised by a polymorph prediction experiment and not all computational job requests can be served in parallel. This leads to demand for additional grid resources

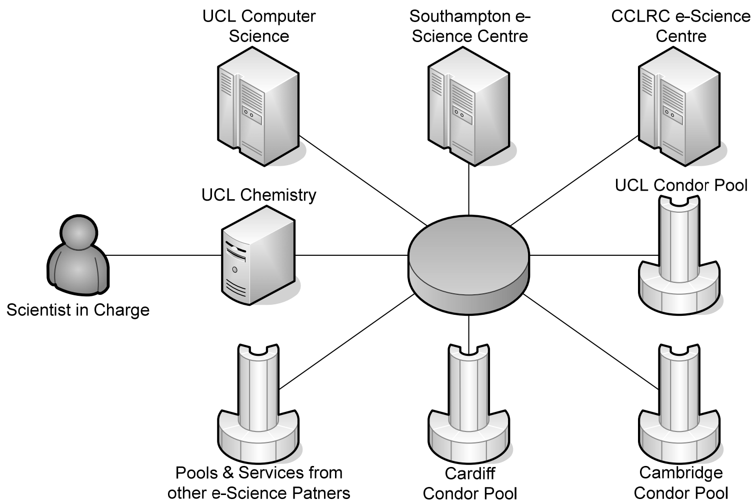

Figure 4.2 –Virtual Lab for Polymorphic Search and Prediction Experiments

(Wilson, Brodholt, and Emmerich 2004). An immediate solution to this problem builds on the transformation of the e-Science laboratory into a virtual organisation that combines the grid resources of scientific organisations in the UK e-Science network as shown in figure 4.2. Federated Condor clusters that are similar to that of UCL, are being provided e.g. by the Universities of Cardiff and Cambridge. Other Condor pools exist at the Universities of Aston, Westminster and Southampton as well as Imperial College. Additionally, a virtual Lab for polymorphic prediction experiments can benefit from various scientific and auxiliary services from members of the UK e-Science network. An example is the utilisation of plotting functionality from the University of Southampton e-Science Centre. Another potential function to be integrated is publication of experimental result data via scientific mediator facilities such as the CCLRC data portal (Drinkwater et al. 2003). A framework of mutual agreements in context of mostly national e-Science initiatives provides the strategic network from which to initiate virtual organisations to run specific experiments.

4.3 Variation of Polymorph Prediction Experiments

General polymorph prediction experiments vary in terms of completeness and precision. Exploratory experiments serve to identify interesting candidates for further examination. They consider fewer packing-alternatives and compute physical properties with less precision. Probing experiments have the purpose of accurately predicting single polymorphs. They need to consider all possible packing-variants and compute properties as exact as possible.

Different types of experiments make similar functional requirements on virtual laboratories, but non-functional requirements vary. Deep experiments require the highest possible level of computational throughput performance. A virtual lab can achieve this by involving as many grid pool providers as possible and delegating as much as possible workload to them. Broad experiments demand less computational performance but a higher level of agility to set-up and run experiments of a series with minimum delays. A virtual lab can obtain this quality by simplifying coordinative regulations and minimising participating grid pools, thus lowering administrative overhead.

We also mention varying requirements of confidentiality, trust and security depending on different research subjects and contexts. E.g., research in pharmaceutical context must not reveal details of possibly highly confidential molecule data. The virtual lab must therefore adjust its administrative procedure to prevent access to experimental data by unauthorised parties.

5. CASE STUDY: VIRTUAL E-SCIENCE SERVICES

We will now use the e-Science scenario for a case study, in which we apply the PARIS reference model to analyse coordination aspect of polymorph prediction experiments and to create a specific VO model for planning and control of individual virtual laboratories.

Initially, we will use the PARIS model to analyse polymorph prediction experiments in terms of points, where regulating and enforcing coordination of cooperative activities between participants of a virtual laboratory is necessary. Subsequently, we turn those points of coordination into parts of a virtual service process. We also identify roles and functions to plan and control polymorph prediction laboratories as virtual production networks for scientific services. These VBSPNs consider variants and variable requirements of specific polymorph prediction experiments.

5.1 Analysis and Modelling of Experiment Processes

The first step towards virtualisation of polymorph prediction laboratories is to analyse the coordination aspects of the experiments they shall carry out. Our method to do so is by structuring the experiment process into components of a virtual business service process. As to this, the PARIS model proposes the concepts of assets, capabilities and demands.

In terms of *assets*, which represent core competencies of providers to produce content, polymorph prediction laboratories predominantly consist of computations in the form of *grid jobs* in general and *MOLPAK* and *DMAREL jobs* in particular. Additional assets include *scientific services* like graph plotting, *(meta-)data publishing* and *auxiliary services* like result data transformation.

Regarding *demands* of polymorph prediction experiments, which represent client side activities to consume service content, we identify the *specification* of experiment subject (i.e. definition of molecule) and parameters (e.g. types of packing and accuracy of properties), *monitoring* of the experiment, *assessment* of result *visualisation* and *download* of result data.

The remaining parts of the virtual service process fall into the category of *capabilities*, which represent administrative procedures to coordinate cooperation of assets and demands for service provision. The first type of *local capability* relates to coordination aspects of individual assets. In polymorph prediction experiments, this translates to coordination of cooperation with grid pools and services. In particular, we identify the need for local capabilities to coordinate *grid job submission, result transformation, result visualisation* and *dissemination management.*

The second type of *global capabilities* relates to coordination aspects between assets and interconnects local capabilities. In the scenario, we identify respective capabilities to coordinate series of MOLPAK and DMAREL computations with

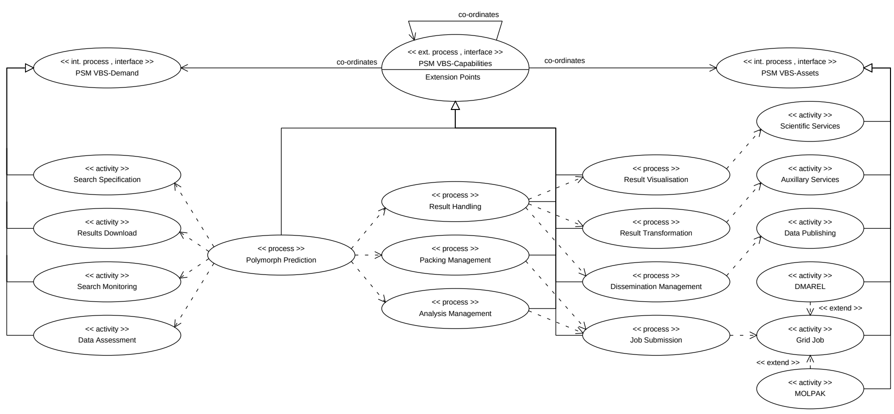

Figure 5.1 – Polymorphic Prediction Experiments as Virtual Service Process

respect to *management of molecule packing* and *packing analysis* in an experiment. We also identify the need for a capability to coordinate scientific and auxiliary services as regards *handling of results*. Finally, a top-level *polymorph prediction capability* needs to coordinate service provision aspects and demands.

The identified components make up a *virtual scientific service process* that captures the coordination aspects of polymorph prediction experiments as ICT-based interaction processes. In figure 5.1, we model the process by means of use cases that extend respective concepts of the PARIS model. We use additional dependencies to denote relationships between capabilities and the components they coordinate.

5.2 Planning and Control of Virtual Laboratories

Based on the analysis of polymorph prediction experiments and their modelling as virtual service process, we now continue following the reference model to shape the organisational structure of virtual laboratories. The way to do so is by modelling the lab as a virtual service production network. We therefore identify various specific roles that we deduce from general roles of the reference model. General responsibilities to plan and control the virtual service process of polymorph prediction experiments translates into the ability to regulate and enforce coordination of cooperative activities between participants of a respective virtual laboratory. We show this first for control and thereafter for planning.

Controlling Experiments

Figure 5.2 shows the components that we have already identified as parts of a virtual scientific service process. In particular, the diagram puts them in association with roles of a specific virtual service production network that we deduce from the three basic role categories of the reference model.

The first role category is the provider, which represents responsibility for realisation of assets including provision of the assets themselves as well as control of local capabilities. With respect to its specific assets, a virtual lab firstly needs the role of a *grid job manager* for realising general job submission in Condor pools and refined roles of *packer* and *analyst* for realising MOLPAK and DMAREL computations therein. Roles realising assets that relate to secondary services include *scientific service provider* and *data portal owner* for result visualisation and dissemination. We also identify the central role of a *polymorph prediction service provider.* On the one hand, this role is a provider of various auxiliary services like data transformation in the course of experiments. On the other hand, this role is also a broker who governs virtual laboratories in the e-Science network.

The second general category of roles is the broker, which represents responsibility for control of global capabilities. Based on the global capabilities of the virtual polymorph prediction service process, we identify the roles of four coordinators with respect to the aspects of managing molecule packing and crystal analysis, handling result data evaluation and running the overall experiment. However, these roles commonly appear in combination with a provider role. We therefore model them as abstract and capture logical combinations with provider roles as refinements. Note, that different such combinations are possible. Specific experiments need to have

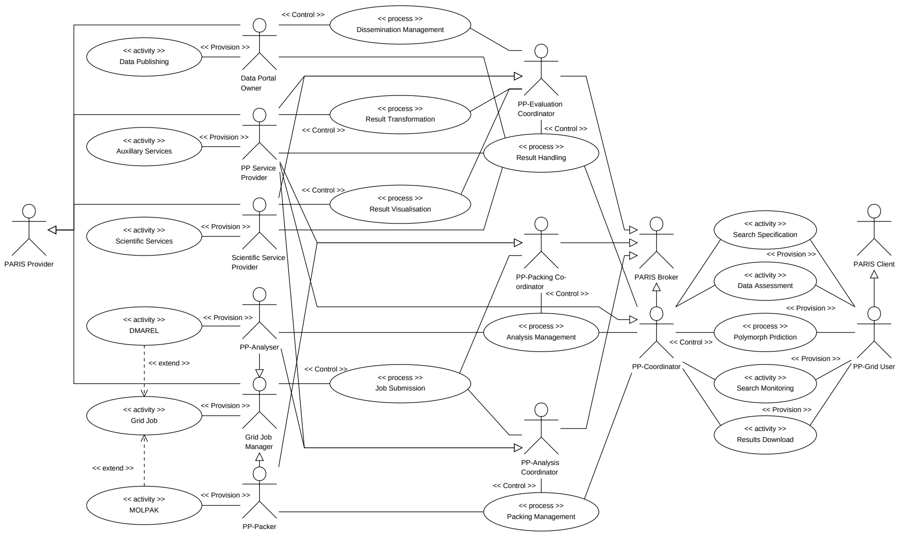

Figure 5.2 – Virtual Polymorphic Prediction Lab Control

exactly one refinement for each role. As we will see, different choices may correspond to experiment variations and their different requirements.

The final role category is the client, which represents responsibility for ‘provision of demands’, meaning active consumption of results. For polymorph prediction experiments, all demands of the virtual service process relate to the scientist in charge. This translates to the more technical role of *polymorph prediction grid user*, which goes along with the responsibility to provide demands in some form of human computer interface.

Planning experiments

After identifying the roles of a virtual laboratory as well as their responsibilities with respect to control of experiments, we now turn to planning of experiments. The reference model defines responsibilities of roles in terms of planning virtual service processes. This includes development of assets as well as development, sighting and adjustment of local and global capabilities. Because we identified the roles of a virtual laboratory as refinements of the generic roles, we already know their responsibilities in terms of planning in general. Yet, the fact that many roles are combinations of providers and brokers demands for further clarification. We mentioned earlier that this has the genuine purpose to allow shifting responsibilities for control of global capabilities between provider roles in order to meet different non-functional requirements of experiment variations. This however does not mean that providers also share responsibility for planning global assets: During investigation, we learned that planning the general method of the experiment is very much in the hand of the scientist in charge and mostly done in association with the role of general service provider for polymorph prediction experiments. We reflect this in our model by re-

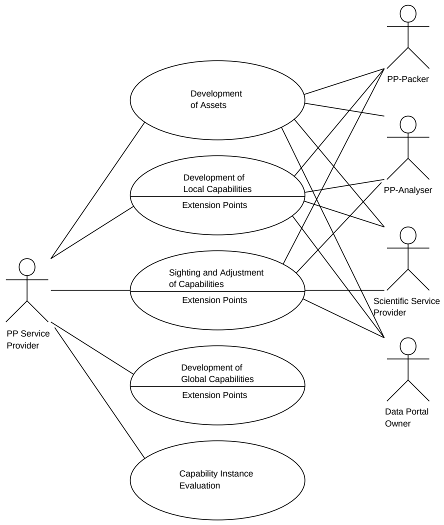

Figure 5.3 – Virtual Polymorphic Prediction Lab Planning

stricting global planning activities to this role. Accordingly, provider roles that relate to grid resources or scientific services only need to plan activities for assets and local capabilities. Figure 5.3 shows these responsibilities between derived roles of a virtual lab and planning related activities of the conceptual model.

5.3 Modelling Experiment Variation with Patterns

The final aspect of the case study is about capturing variations of polymorph prediction experiments and translating them into an organisational structure of virtual laboratories that shows sufficient degrees of flexibility and agility. For this purpose, the PARIS model offers the concept of pattern-based regulation. In particular, this includes regulating coordination of cooperation by means of interaction patterns and regulating enforcement of coordination by means of orchestration idioms.

Interaction patterns in the virtual laboratory scenario correspond to VBS capabilities of polymorphic prediction. Figure 5.4 lists them on the right. From an organisational perspective, they restrict interactions between participants in terms of content and causal/temporal properties. They do however not restrict the enforcement of such regulations in terms of necessary orchestration activities and assignment of responsibility for their execution. Thus, we separate the general principle of coordination, which always remains the same, from the specific mechanism of enforcement, which is different for each variation of the experiment. For instance, the packing management pattern includes interactions of MOLPAK parameters from the grid user to polymorph prediction packers and subsequent interaction of results in the reverse direction. Additional regulations ensure eventual interaction of consolidated results to the next stage of analysis management and so forth.

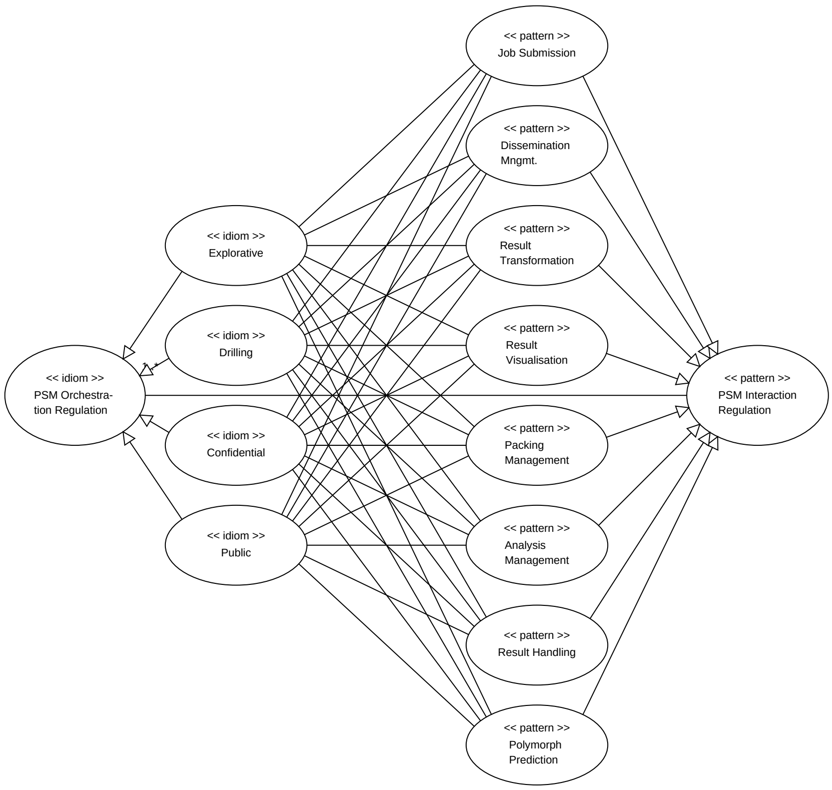

Figure 5.4 – Patterns of Polymorphic Prediction Experiment Variation

Conversely, orchestration idioms correspond to non-functional requirements of experiment variations for polymorph prediction. Figure 5.4 lists them on the left. Each of the idioms captures a distinct strategy to implement the enforcement of general interaction patterns by translating them into specific orchestration procedures and assigning executive responsibilities to specific lab roles. The design of implementation strategies mirrors requirements of experiment variations and translates into non-functional properties of resulting organisational structures. We outline their strategies on organisational level for experiment variations as follows:

- *Broad* (series of approximating experiments requiring agility): Implementation strategy translates interaction patterns to orchestration activities of single consolidated capability enforcement instances for centralised execution by polymorph prediction service providers. The goal is to minimise deployment and interaction between global capabilities.

- *Deep* (single detailed experiment requiring throughput performance):
  Implementation strategy translates interaction patterns to orchestration activities of many interrelated capability enforcement instances for decentralised execution by a maximum number of providers. Load balancing of global capabilities results in optimised performance and scalability.
- *Confidential* (experiment on classified subject requiring confidentiality):
  Implementation strategy translates interaction patterns into orchestration activities of few interrelated capability enforcement instances for execution by a set of trusted providers. Limiting data visibility and reducing interaction of global capabilities minimises risk of disclosure.
- *Open* (cooperative experiment requiring transparency):
  Implementation strategy translates interaction patterns into orchestration activities and combines them into a general capability enforcement instance for replication and execution by all providers. Sharing of procedure and state between global capabilities maximises individual insight.

Combination of patterns and idioms results in the desired effect on virtual laboratory organisational structure. Once that regulation of patterns and idioms are finished in a one-time effort, it is possible to adjust organisational structure of virtual laboratories for each experiment individually. Based on one or more variants, respective idioms allow for transformation of interaction patterns into procedures and assignments of orchestration-based enforcement that result in optimised organisational structures with adequate non-functional properties.

6. VIRTUAL SERVICE IMPLEMENTATION

In this paper, our focus is on organisational level. We have therefore introduced concepts in terms of their organisational properties rather then their technical implementation. However, the organisational properties vitally build on ICT to enable them. Pivot point between these levels is the idea of business service virtualisation for the benefit of business service production management.

Accordingly, a major step for implementing our conceptual model concerns service virtualisation technology. We need to point out that actual implementation of VBSPN concepts in business context is a complex task, which involves a multitude of aspects on various levels of a holistic enterprise architecture framework. Our work however concentrates on implementation of technology aspects.

Therefore, the initial task is to deduce requirements for service virtualisation technology. We will then classify such technology in the context of ICT infrastructure for virtual organisation and identify base-technologies to build on. In particular, we will assess utilisation of service-oriented technology.

6.1 Requirements for Business Service Virtualisation Technologies

The PARIS model presents an approach to regulate and enforce coordination of cooperative activities by participants of a strategic network that is flexible and agile enough to enable mission-specific virtual organisations. The approach builds on an organisational strategy that regulates and enforces coordination of clients and providers within a service production network by planning and controlling their interactions during service process operation. The organisational strategy in turn builds on a technical strategy of business service virtualisation. It supports organisational planning and control tasks with ICT-based methods that operate on ICT representations of service process interactions. Thus, technical requirements for ICT representations and ICT based methods used for service virtualisation go back to organisational prerequisites for interaction-based coordination of VO structures.

Prerequisites of Organisational Concept

Fundamental to the PARIS approach is a perspective, which perceives organisational missions as (business) services provided by virtual organisations as virtual service production networks (VBSPN). This perspective focuses on the service process, which includes activities of participants involved in a mission and is inherently interactive. During service production, coordination of participants corresponds to the flow of their interactions in the service process. This relationship translates into a strategy to regulate and enforce coordination. We achieve regulation of coordination by planning interactions as programs, whereby planning of programs relies on plans to ensure meeting requirements of flexibility and agility. In turn, controlling interaction programs leads to enforcement of coordinative regulations.

In the organisational structure of virtual service production networks, regulation and enforcement of coordination translates to tasks of service production planning and control on network- and node-level. On network-level, brokers plan interaction (process) patterns between clients and providers as programs to regulate coordination. They also plan a structured procedure for the planning task itself. Subsequently, coordinators control interaction flow between clients and providers as planned by patterns to enforce coordinative regulations. Likewise, on node-level, clients and providers plan communication endpoints to their internal processes as programs to regulate their coordination. Again, they also plan a structured procedure for the planning task itself. In operation, they control communication with their internal processes as planned by the communication endpoints to enforce coordinative regulations.

Requirements for VBS Technology

In VBSPNs, service virtualisation fundamentally facilitates the tasks of service production management. It entails ICT-based substitution of conventional interaction within service processes, resulting in virtual business service processes (VBSP). In particular, ICT representations of interaction processes substitute interaction patterns of service processes. ICT representations of interfaces substitute communication endpoints of service process activities. Virtualisation enables ICT-based methods in the different service phases that are applicable for production management tasks in turn.

Preparation of VBSPs in the service pre-contact phase needs methods for explicit design, formal specification and mutual adjustment of virtualised interaction patterns and endpoints. These methods facilitate tasks of interaction program planning on network- and node-level of VBSPNs. They require formal process and communication models as well as standardised languages for protocol and interface specification. Operation of VBSPs in the service contact phase needs methods for automated execution of virtualised interaction patterns and communication with virtualised endpoints. These methods facilitate tasks of controlling interaction flow and communication on network- and node-level of VBSPNs. They require programming models and runtime mechanisms of inter-enterprise process and middleware platforms for execution of interaction processes and interface communication as well as mechanisms to construct executable process representations. Analysis of VBSPs in the service post-contact phase needs methods for evaluation and possible change of virtualised interaction patterns and endpoints. These methods facilitate tasks of (re-) planning interaction patterns and endpoints on network- and node-level of VBSPNs. They require runtime monitoring and formal methods of software system evolution.

Generally, methodologies are needed to superimpose structure on all methods and to allow for formal definition of virtual service development lifecycle processes. They facilitate tasks of planning structured procedures for the planning tasks themselves on network- and node-level of VBSPNs. This requires consideration of meta-models to allow for formal specification of development processes.

6.2 Implementation of Business Service Virtualisation Technologies

We now wrap up the findings in a brief characterisation of general service virtualisation technologies. Thereafter, we classify such technology with respect to generic information technology infrastructure of virtual organisations. Finally, we assess service-oriented technologies as possible basis for implementation.

Service virtualisation is about utilising information and communication technology for the benefit of coordinating VBSPN participants. This requires service virtualisation technology (a) to represent and (b) to manage VBSPs.

Representation of VBSPs relates to virtualised interaction patterns and communication endpoints. Both aspects need coverage as model, design, architecture, executable and audit trail for application software systems of participants. *VBSP representation technologies* provide means to implement VBSPs as coordinated flow of communication activities between operative application software systems belonging to VBSPN participants for the benefit of integration into an inter-enterprise cooperative information system that serves for control of service production.

VBSP management relates to the business service phases of preparing, operating and analysing VBSPs. Theses phases build on methods for design, adjustment, verification, construction, testing, deployment, execution, monitoring, analysis and evolution of VBSP representations. Generally, *VBSP management technologies* subsume development processes and methods for VBSP representations that conform to flexibility and agility requirements for instant planning of VBSPNs.

Classification of Service Virtualisation Technologies

Information and communication technology (ICT) is widely regarded as key enabling factor for virtual organisations and considerable research has focused on this aspect of the ICT subsystem of business information systems (Camarinha-Matos and Afsarmanesh 2003). As a result, common functional patterns have been identified for ICT infrastructure of virtual organisations (Camarinha-Matos 2005). Table 6.1 shows according functional categories of virtual organisation ICT infrastructure.

Infrastructure for B2B-integration in VBSPN

Infrastructure catagories		
Horizontal base-infrastructure	Communication	Connectivity
		Security
		Interoperability
	Cooperation	Coordination
		Info- & knwldg. sharing
		Collaboration
Vertical functions in VBSP-lifecycle	Initiation	Breeding environm. / electr. service market
	Operation	Distributed business processes
		Domain functions
	Liquidation	After sales services, knowledge mngmt.
Non funct props		Standardisation
		Agility
		Flexibility

Aspects of business service virtualisation technology

VBSP-representation technology		Base Technology (BT)	SOA/SOC areas & concepts	WS Technology	WS Standard
Communication	(Meta-) models and methods for **communication endpoints of production units** to enable planning and control				
	(Meta-) models and middleware for **software components** to enable component specification and interaction	Mechanisms for publishing interface descriptions	Service-oriented system integration: Discovery & selection via registries	WS Brokerage	E.g. UDDI
		Standard languages for interface description	Description & Publication via IDL	WS Description	E.g. WSDL
		Mechanisms for interface communication	Binding & interaction via P2P-middleware	WS Access	E.g. SOAP
Coordination	(Meta-) models and methods for **interaction patterns in service processes** to enable planning and control				
	(Meta-) models and IT-platforms for **interaction processes** to enable protocol specification and execution	Process representation as coordination protocol	Service-oriented process integration: Regulation of collaboration via coordination protocols	WS Coordination	E.g. WSCI
		Execution of process representations based on interface communication	Implementation of coordination rules via composition schemas	WS Composition	E.g. BPEL

VBSP-management technology		Base technology (BT)	SOA/SOC areas & concepts
Development methods	Structured methods for **formal design** and **mutual adjustment** of interaction patterns and communication endpoints	**Structured methods** in development lifecycles of VBS base technologies	Service-oriented development methods: Service-oriented analysis and design methods
	Structured methods for **automated control** of interaction patterns and communication endpoints		Service construction, testing, provisioning deployment and execution methods
	Structured methods for **formal analysis** and **systematic change** of interaction patterns and communication endpoints		Service monitoring methods
Methodology	Provision of a structured **VBS-methodology** for ad hoc coordination of production units in VBSP		
	Generic **Frameworks** as well as technology specific **methodologies** and **development processes**	BT	Service-oriented development lifecycle methodology

Table 6.1 – Service-Oriented Technology for VBSPN ICT Infrastructure

The schema separates horizontal infrastructure to enable generic functionality of communication and cooperation from vertical infrastructure to enable (domain) specific functionality to support lifecycle phases of virtual organisations. Communication technologies for virtual organisations need to consider fundamental connectivity, systems interoperability as well as security. Cooperation technologies include mechanisms to share information and knowledge, techniques for unstructured collaboration as well as more structured approaches of coordinated cooperation. Lifecycle support includes general phases of initiation with aspects like breeding and network-internal markets, operation that strongly relates to distributed business processes as well as liquidation that concerns e.g. after sales services and knowledge management. Furthermore, we mention non-functional aspects of standardisation, flexibility and agility as complementary aspects of ICT infrastructure.

VBSP representation and management combine multiple aspects of generic virtual organisation ICT infrastructure in the light of business service virtualisation. We will now classify subsumed technologies under general categories as fundamental ICT infrastructure components of virtual service production networks. This will reveal overlap with base-technologies as well as specific parts that need to be implemented individually.

We generally classify VBSP representation technology as integration technology of horizontal base infrastructure. Focal points are interoperability and coordination. In terms of interoperability, VBSP representation technology provides models and mechanisms for planning and controlling communication endpoints of VBSPN participants. They build on base-technologies of middleware platforms that allow for inter-enterprise specification and communication of software components. In terms of coordination, VBSP representation technology provides models and mechanisms for planning and controlling interaction patterns of VBSPs. They build on base-technologies of process platforms like inter-enterprise workflow systems that allow for protocol specification and execution of interaction processes. Connectivity and security, Information sharing and collaboration are considered important complementary aspects outside service virtualisation core technology.

We classify VBSP management technology as vertical infrastructure to support the VBSPN lifecycle. Methods to develop VBSP representations provide functionality to support management tasks in the lifecycle phases of VBSPNs. Regarding general categories of functionality, VBSP management technology relates to distributed business process support, which it provides over the whole lifecycle. During VBSPN initiation, methods for formal design, verification and adjustment of interaction patterns and communication endpoints support production-planning tasks. In VBSPN operation, methods for construction, testing, deployment, execution and monitoring of respective integration mechanisms support production control tasks. Finally, for VBSPN liquidation, methods for analysis of operation and evolution of design provide additional support for production-planning tasks. All methods may benefit from and integrate with existing development methods of VBSP representation base-technologies.

Complementary aspects of service virtualisation technology relate to intrinsic requirements on flexibility and agility of mission-specific VBSPNs. To cope with these, VBSP management methodology governs planning of production management tasks by means of structured development lifecycle processes. Here, base-technology comes in form of generic reference models and frameworks as well as specific methodologies and development processes of VBSP representation base-technologies.

Business Service Virtualisation Based on Service-Oriented Technologies

As service virtualisation technology overlaps generic VBSPN ICT infrastructure to a large extend, the choice of base-technology is vital to its implementation. As to this, a variety of technologies, including distributed object-, component-, agent- and service-oriented software technologies and middleware platforms broadly fulfil the requirements. However, shared conceptual roots of generic service theory underpin the assumption of an above average level of support to be gained from utilisation of service-oriented technologies.

Web Services, as predominant technology to implement the SOC paradigm, allow inter-enterprise representation of business interactions as well as access to encapsulated intra-enterprise processes and information systems (Alonso et al. 2004). On top of this basic abstraction, a variety of integration mechanisms allow for operating atomic interactions as well as for regulating and implementing complex interaction processes. The design of these mechanisms considers requirements of inter-enterprise contexts, which includes decentralisation of critical aspects by peer-to-peer middleware protocols. Moreover, global and successful standardisation led to widespread use. Overall, SOC and especially WS technologies open up benefits of integrative middleware to the inter-enterprise context of VBSPN.

Conceptual similarities encourage utilisation of WS technologies for business service virtualisation and show ways to do so. The fundamental service-oriented model defines provider and client roles that are responsible for implementation and access of software services. They match respective roles of our business service model that prepare and operate business services. Furthermore, roles of client, provider, broker, aggregator and operator in the extended service-oriented model, which considers composed and managed software services (Papazoglou and Georgakopoulos 2003), are closely related to the roles of production units, coordinators and brokers in the organisational VBSPN model. In this constellation, utilisation of software service technologies to describe, publish, discover, bind, access, coordinate, compose and manage software services in the software service development lifecycle offers opportunities for organisational virtualisation of VBSPN.

Following these conceptual similarities, the lower part of table 6.1 shows a possible mapping of VBSP representation and management technologies to service-oriented base-technologies. Regarding VBSP representation, the mapping shows service-oriented base-technologies for interoperable communication as well as regulation and enforcement of coordination. Software services naturally provide an implementation of communication endpoints. They offer ways of description (e.g. WSDL) and interoperable access (e.g. SOAP) as well as additional support for the planning task by means of brokerage (e.g. UDDI). Technologies for software service interaction processes provide basic mechanisms to implement interaction patterns. This includes service coordination regulation via interaction protocols (e.g. WSCI) and implementation of regulations via service composition techniques (e.g. BPEL).

Regarding, service-oriented base-technologies for VBSP management, some early results of software service development methods and processes are already available for utilisation. Papazoglou et al. proposed a service-oriented development lifecycle methodology (Papazoglou and van den Heuvel 2006) that shows considerable similarities to VO lifecycle models like that introduced by Mertens et al.

(Mertens, Griese, and Ehrenberg 1998). Software-service development methods include several categories of VBSP management technology requirements. An overview can be found in (Papazoglou and van den Heuvel 2006). An area of specific interest for VBSP management is flexible design of VBSP interaction patterns and agile construction of executable VBSP representations. As to this, software service development methods of potential benefit include those that offer rule-based and model-driven approaches. E.g., Orriëns et al. proposed a method for rule-based construction of software service composition schemas (Orriëns, Yang, and Papazoglou 2003) and a rule-based software service development framework for collaborative information systems (Orriëns, Yang, and Papazoglou 2005). Colombo et al. proposed a method for pattern-based modelling and analysis of software service compositions (Colombo, Mylopoulos, and Spoletini 2005). We also note graph transformation-based methods for context aware software service composition by Baresi et al. (Baresi et al. 2003; Baresi, Maurino, and Modafferi 2005).

7. RELATED WORK

The research-area of virtual organisation and collaborative networks has been gaining considerable momentum over recent years (Camarinha-Matos and Afsarmanesh 2004). To the best of our knowledge, the approach of organisational business service virtualisation based on service-oriented software technologies is unique. Yet, the work of several projects from the research communities of enterprise engineering (e.g. around GERAM), virtual and network organisation (e.g. around PRO-VE, VOSTER, ECOLEAD) as well as database and software technology (e.g. around ICSOC and NESSI) led to results overlapping with parts of ours. In the following, we describe links to related work as regards 1) VO concepts and modelling, 2) VO models based on business services, 3) models of organisational virtualisation based on software services and 4) virtual organisation of research laboratories.

7.1 Virtual Organisation Concepts and Modelling

The most elemental foundation of our work is the VO concept itself. As a wider consensus about virtual and other forms of network organisation has been a gradual achievement of the last decade, we shall define a respective point of reference first. Primarily, we refer to the basic concepts covered by economical perspectives and base our fundamental understanding of VO on reference models like that proposed by (Katzy, Zhang, and Loeh 2005). The PARIS conceptual model specialises these fundamental aspects towards more specific aspects of virtual production networks for business services. In the schema of Katzy, the characteristics of these networks resemble those of *supply chains* overlaying *hub-and-spoke* structures.

In more practical terms, the multitude of aspects that one needs to consider for VO calls for multiple models with different purposes and perspectives as well as on different levels of abstractions and for different audiences. In order to classify our own modelling approach, we refer to VO modelling frameworks that were proposed for this purpose by (Loeh, Zhang, and Katzy 2005) and as part of the **ARCON** reference model (Camarinha-Matos and Afsarmanesh 2006). With respect to the modelling framework of Loeh, the PARIS conceptual model has the purpose of explaining our general approach to organisation and its technical virtualisation. It is an *en-*

terprise engineering type model that serves as a guideline to specify models of virtual organisations in concrete scenarios. These are *system requirement models* with the purpose of describing specific forms of VO and their implementation by means of ICT infrastructure. Following the argumentation of Camarinha-Matos, the PARIS conceptual model classifies as *enterprise engineering reference model* for virtual business service production networks. In ARCON terminology, it mainly describes the inside perspective of organisation in terms of structural, functional, componential and behavioural perspectives on a general concept level. The outside perspective is present with aspects of market and support dimensions.

7.2 Service-Based Modelling of Virtual Organisations

Turning to specific approaches, a number of projects in the abovementioned areas proposed conceptual VO models that somehow relate to an economic notion of service. From the area of enterprise engineering, the **GLOBEMEN** project proposed, among many other things, a reference model that refers to a similar type of service-based VO then PARIS. The *virtual enterprise reference architecture (VERA)* (Vesterager, Tølle, and Bernus 2003) includes *service virtual enterprises (SVE)* as a distinct type of virtual enterprise for service production matters that are part of more general production missions for one-of-a-kind products (Jansson, Karvonen, and Ollus 2003). SVE services build on a collaborative service reference model (Hartel and Burger 2003) that adopts GERAM principles (IFIP–IFAC 2003) and targets primarily management aspects. It is not concerned with service virtualisation or service-specific coordination approaches. Compared to PARIS, SVE and the collaborative service reference model offer a complementary approach on management level and underpin the relevance of a business service-based perspective.

In an approach from the area of service engineering, the **FRESCO** project investigated system requirement models of *business service collaboration* and their implementation based on service-oriented middleware (Zirpins, Lamersdorf, and Piccinelli 2004). The focus is on supply chain organisation of b2b e-Commerce scenarios that builds on a process-based model of business service collaboration. A service-engineering platform offers lifecycle support for definition, enactment and evolution of *collaborative services*. The platform implementation adopts Grid and Web Service interaction process technologies. PARIS adopts experiences with business service modelling in FRESCO. The PARIS conceptual models provide organisational background, refine the service model and leverage it on business level.

An example of an infrastructure approach from the database area, that employs a system requirement model of business services, is the **CrossFlow** project (Grefen et al. 2000). Its background is the dynamic outsourcing of a part of the business process of a company to another company that provides this part as a service. The resulting bilateral supply chain organisation builds on *service contracts*. A cross-organisational workflow platform layer supports contract establishment, infrastructure configuration, contract enforcement and infrastructure disposal. The system requirement type service process model is typical for technically biased infrastructure approaches. In comparison, the PARIS service process model offers the benefit of an organisational dimension to embed technology in the enterprise architecture.

To complete this list, we mention the VO coordination approach in **PRODNET II** (Camarinha-Matos and Pantoja-Lima 2001) that builds on a complex process model and shows similarities to PARIS virtual service processes. The process structure includes services as abstractions for coordination functionality on different hierarchical levels. The coordination approach materialises as an infrastructure layer that provides mechanisms to define and enforce coordination processes. The PARIS conceptual model shows similarities in terms of its structural process modelling approach of virtual service processes and capabilities. It differs in its focus on organisation of coordination management that complements the PRODNET approach.

7.3 Virtual Organisation Models Based on Software Services

From a more technical perspective, *service federation* emerged as a paradigm that serves well for modelling VO structures as well as for the realisation of ICT infrastructure by means of service-oriented software technology (Camarinha-Matos 2005). In VO modelling, software services represent shared assets and focus their peer-to-peer access within strategic networks. Software service compositions represent supply chains and focus their distributed business processes. An aggregator role constitutes a central point of responsibility for software service brokerage and composition tasks. This model particularly matches scenarios of industry cluster integration. Moreover, common standard languages and protocols as well as availability of COTS-middleware render implementation feasible for SMEs. Conforming to this paradigm, PARIS adopts software service abstractions for representation of distributed business processes and offers a comprehensive framework of organisational concepts that describes how to utilise software service lifecycle methodology to support dynamic coordination of VO business process chains.

We shall briefly mention some projects that adopt VO modelling approaches, using respective abstractions of software service and software service composition. One such project is **WebBIS** (Benatallah et al. 2000) that employs a system requirement type service model with rule-based coordination concept. It introduces *virtual enterprise services* that specify and enforce their individual coordination logic by means of ECA rules. They group in *communities* that resemble a peer-to-peer virtual organisation type. We consider the rule-based approach to coordination particularly versatile but note that transition to management level might be difficult. The PARIS approach offers a medium-grained process structure instead.

A higher level service model is proposed within **CMI** (Georgakopoulos et al. 2002). Here, *e-Services* build on a model of *service-oriented processes (SOP)* for behavioural description. SOPs also model supply chain type VO as *multi-enterprise processes (MEP)* that integrate and coordinate e-services and are executable by means of the *collaboration management infrastructure (CMI)*. Overall, CMI introduces sophisticated models of system behaviour, but a transition path towards management type modelling and organisation of coordination tasks is not part of the project. Such a path is subject of the PARIS conceptual model.

The **WISE** project (Lazcano et al. 2000) proposed a service federation approach that not only considers system requirements but also management type models. It introduces *virtual business processes* to integrate *services* of members in *trading communities* that resemble supply chain type VO. Integration follows a higher-level context of regulations named *virtual enterprise*. A workflow-based ICT infrastructure layer supports definition, enactment, monitoring and analysis of virtual business processes as well as some unstructured forms of communication and coordination.

Overall, WISE offers a process-based structural and lifecycle model of virtual enterprises. PARIS focuses on a refinement of similar models as regards business service production and offers a more detailed organisational model of VO coordination.

The last project to mention here is **Fetish-ETF** (Camarinha-Matos et al. 2001). It follows a peer-to-peer type VO approach for service providers of a tourism industry cluster. A *promoter node* utilises service market mechanisms for virtual enterprise initiation. He promotes services either in *atomic* form or as *value added services*. The latter build on general distributed business processes. An ICT infrastructure supports the organisational approach by mechanisms including service interaction, catalogues and workflow-based composition. This approach appears to work well for the specific domain that it targets. While following these lines, PARIS proposes more versatile process and organisational models for VO coordination.

7.4 Organisational Virtualisation of Research Laboratories

As regards our case study, the concept of *virtual laboratory* was also subject to prior investigation. Generally, the domain of e-Science calls for specific collaborative networks in form of heterogeneous, distributed problem solving environments that enable groups of researchers located in different geographical places to work together and share resources like equipment, tools and data (Camarinha-Matos 2005). This typically requires ICT infrastructure to support remote operation, information management, simulation and collaborative tools. PARIS-based e-Science targets a narrower perspective of coordination management for structured experiments. The focus is on structured scientific processes of remote operation and information management as well as their management in virtual organisations.

An Example of a general problem-solving environment to support research collaboration is the **Virtual Laboratory** (VL) project that proposes a *reference architecture for scientific virtual laboratories* (Afsarmanesh et al. 2001). It supports loosely structured collaborations of researchers in peer-to-peer type VO and mainly considers requirements like management of large data sets, information sharing for collaboration and distributed resource management. This approach is more general and covers different scenarios then the PARIS case study. Likewise, it does not address the specific problems and requirements of coordinating polymorph prediction labs that are covered in the PARIS solution.

In contrast to such collaborative environments, we finally mention an approach to workflow based e-Science. The **Sedna** environment offers support for structured experimental processes (Wassermann et al. 2007). Fundamentally, it proposes an architectural approach for high-throughput computations by means of software service composition. A toolset supports design and deployment of scientific workflows as orchestrations of grid and web services. *Scientific workflows* build on a model of structured scientific experiment processes. The approach showed its feasibility in a successful case study for polymorph prediction e-Science. The Sedna approach underpins e-Science support by structured experimental processes in the PARIS example scenario. So far, it does not consider organisational aspects or application in an inter-organisational context. The PARIS case study provides an extended model that can help to extend Sedna for virtual organisation contexts.

8. SUMMARY AND OUTLOOK

In this paper, we proposed a model for ICT-based regulation and enforcement of coordination for cooperative activities between participants of virtual organisations. The distinctive aspect of our approach is to adopt a service-based perspective on virtual organisation and to exploit benefits that result from high virtualisation potential of interactive service processes. To capture this principle in a concise yet comprehensive way, we made use of conceptual modelling by means of UML use case diagrams. Thereby, we specified our views on business services and production networks in conventional and virtual forms. The conceptual models conclude with virtual service production networks that fulfil flexibility and agility requirements of virtual organisations. Virtual business services anticipate multiple variants to enforce general coordinative regulations and capture these as orchestration idioms of interaction patterns. This allows for ad hoc optimisation of non-functional properties based on mission-specific requirements.

We illustrated the practical application of our model for domain analysis by example of a case study on organisational virtualisation in computational chemistry e-Science. Based on current practice of computational polymorph prediction research and experiments, conceptual categories of the PARIS model helped analysing interaction structure as well as identifying coordinative dependencies and their variations. The result was a specific conceptual model for organising planning and control of virtual polymorph prediction laboratories. In particular, the organisational structure anticipates variants of broad, deep, confidential and open polymorph prediction experiments and allows ad hoc adjustment of operational interaction process chains for rapid initialisation of mission specific virtual laboratories.

Finally, we outlined requirements, categories and candidates for ICT to implement our model concepts. Fundamentally, we explained, how organisational requirements of virtual business service production networks lead to technical requirements for business service virtualisation technology. Here, we identified representation and management of business service processes as key technologies. They implement organisational management tasks of service production planning and control through agile development of flexible cooperative information systems. We then showed how these technologies fit in the general context of ICT infrastructure for virtual organisations and how they overlap with fundamental functionality to support implementation. In particular, analysis of service-oriented base-technologies revealed conceptual similarities that promote utilisation of Web Service base architecture, coordination and composition as well as software service development lifecycle methodology and mechanisms.

In our ongoing work, we are following the outlined path of organisational virtualisation based on service-oriented technology. An immediate activity is to develop metamodels of interaction and orchestration patterns for business service process representation based on software service abstractions. We are also specifying a software service development lifecycle methodology for business service process management. As for respective development methods, our priority is on model-driven construction of orchestration processes by rule-based transformation of interaction patterns.

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