From ad-hoc modelling to strategic infrastructure: A manifesto for model management

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From ad-hoc modelling to strategic infrastructure: a manifesto for model management

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Abstract

Models are playing an increasingly prominent role in watershed management, and environmental management more generally. To successfully utilize model-based tools for governing water resources, modelling timelines must match decision making timelines, and modelling costs must fall within budget constraints. Clarity on management options for modelling processes, and effective strategies, are likely to improve outcomes. This paper provides a first conceptualisation of model management and lays out its scope. We define management of numerical models (MNM) as governance, operational support, and administration of modelling, and argue that it is a universal activity that is crucial but often overlooked in organisations that rely on modelling. The paper lays out the leverage points available to a model manager, based on a review of model management practices in several fields, highlights lessons learned, and opportunities for further improvement as model management becomes a mainstream concern in both research and practice.

Highlights

- Emerging explicit knowledge around managing numerical modelling (MNM) processes.
- MNM improves return on investment in model-supported decision infrastructure.
- Leverage points are procedural guidelines, cyberinfrastructure, knowledge management.
- Blue-print approaches to MNM are not expected to be successful.
- Consideration of context important - an agency’s roles, capacity, and resources.

Keywords

Model management; Workflow; Cyberinfrastructure; Knowledge management
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1. From emergent to deliberate management of models

Numerical models used for forecasting and scenario analyses are ubiquitous in watershed and environmental management (Kumar, 2011). Models offer a toolbox of methods to connect data meaningfully, explore non-factual situations, quantify outcomes of system interventions, and facilitate communication about complex science between experts and non-expert stakeholders (Basco-Carrera et al., 2017). While we could conceivably tackle many problems without numerical models, to make statements about the future and evaluate different options, modelling tools typically provide better and quicker information than historical data analysis (Freeze and Harlan, 1969; Fatichi et al., 2016). Under a changing climate, the use of these tools will only increase, to support development of resilient societies (Djalante et al., 2011; Montanari et al., 2013; Marchau et al., 2019). How can models, as essential tools, be utilized efficiently and cost-effectively?

Several guides inform the successful execution of modelling processes. Some organize them along a sequence of technical modelling steps, which may require revisiting earlier steps and lead to circular, iterative or even recursive model formulation (Jakeman, 2006; Badham et al., 2019). Such steps are also reflected in Good Modelling Practices that govern engineering studies, for example background scoping, the documentation and communication of calibration procedures, and the discussion of results and its uncertainty (e.g. Rassam et al., 2011; Refsgaard and Henriksen, 2004; or the ASTM series on groundwater modelling). Other guides describe non-technical success factors of modelling projects such as communication and trust between modellers and stakeholders (Merritt et al., 2017; Hamilton et al., 2019).

However, modelling processes continue to challenge most watershed agencies. One reason is that models are increasingly complex due to the need to capture processes and scenarios with many interacting variables (Mirus et al., 2011, Fatichi et al., 2016). Accompanying documentation can be difficult to interpret and written in technical language for specialists, and complicated IT systems pose another barrier. As a result modelling increasingly relies on new forms of specialist knowledge, driving up the overall cost of model-based decision making. While models are essential tools for water management agencies, systematic development of model-based knowledge- and decision support infrastructure is often not a priority (Marchildon et al., 2018).

In public-sector agencies, formal knowledge about the management of numerical models (MNM) is
slowly emerging (Arnold and Marchildon 2018). Comparing model management with the progress in data management (Horsburgh et al., 2008; Wilms et al., 2018) sheds light on the limitations of model management practices to date. Data management is now a well-defined priority task in almost every environmental agency, often handled in dedicated departments, such that data is standardized, verified, conveniently accessible to all staff, and integrated with analysis and visualization software. In contrast, in most watershed organizations, modelling is neither centrally supported, standardized, nor managed. Only a few agencies, for example those specialized in Earth Sciences (e.g. meteorological and oceanographic services or climate research centres) have institutionalized sophisticated model management practices, while most agencies rely on the ad-hoc decisions of environmental managers (Arnold and Marchildon 2018).

The objective of modeling in watershed agencies is to strengthen the agency’s ability to manage watersheds within available resource constraints, while fulfilling legal duties and social responsibilities. This requires agencies to manage knowledge around models, model implementation, model development, and result communication. Management of numerical models (MNM) therefore encompasses governance, operational support, and administration of modelling: the managerial procedures by which technical modelling projects are governed, 2) the technologies that make up an organization’s infrastructure for data and modelling knowledge and IT support, and 3) the human resource aspects of how knowledge is accessed throughout the model’s lifecycle.

The cost of poor model management practices in public and private agencies is difficult to measure, and lessons on how the returns from “public investment into numerical models as knowledge investment” (Marchildon et al., 2017) could be enhanced are difficult to find, especially because model management is not recognized as an explicit responsibility of agencies.

While MNM is a general issue, this paper specifically focuses on MNM as it relates to watershed management agencies (“watershed agencies” for short) - public or private agencies that govern at watershed level. The aim of this paper is to raise awareness about the role that MNM could and already does play, and about the currently prevailing emergent rather than deliberate MNM in watershed management (Mintzberg and Waters 1985). We first introduce the concept of model management further, introduce the functions and tasks that model managers must enable watershed agencies to fulfill, and derive activities for a model manager. Then, we derive lessons from several fields of practice, in order to derive generic insights into the management of numerical models in watershed
agencies. Finally, we discuss these lessons and identify critical aspects and opportunities for improving current model management practice in watershed management agencies, for better watershed governance. This paper provides a starting point that attempts to bridge academia and practice.

2. Conceptualising model management

2.1. Model management is knowledge management ...

The main currency of modelling is knowledge in its various fields and forms. Modelling processes most orchestrate relevant knowledge fields and overcome departmental and paradigmatic compartmentalization (Arnold 2013). For this, MNM needs to consider human behavior of the people involved, each of whom is embedded in a social context (Hämäläinen 2015, Lahtinen et al., 2017a).

Model management is fundamentally a knowledge management task, but knowledge management is itself a multi-faceted beast, which includes enabling the flow of knowledge between participants; ensuring timely access to, documentation, and archiving of all relevant forms of knowledge; knowledge exchange infrastructure; providing an enabling environment for people with the right skills; mentorship and conflict resolution.

We define an environmental model site application (short “model application”) as one or several software tools that are set up to simulate particular locations and systems using observational data. The core of the model application is a technical modelling process, involving a model code - a software package (or several coupled ones) that perform core tasks of a computer simulation, combining input files, scientific laws and assumptions in order to create output files. For the model, observation data is needed from existing sources, by measurement, or from experts (Seibert and McDonnell, 2002). Pre-processing may be needed to transform data into input data; and post-processing to translate model output into the actual modeling results from which policy and management implications might be derived. In our definition, any software tools used for pre-and post-processing are part of a model application. Model uncertainty is addressed explicitly and implicitly - taking into account the combined impact of all assumptions, omissions and errors, and in the observed data when preparing and presenting study results (Linkov and Burmistrov 2003, Arnold, et al., 2015).

The central purpose of working with model applications is learning about specific environmental systems. In principle, models focus, contextualize and enrich the available system knowledge. Yet, this
requires other fields of knowledge beyond understanding the system at hand. Regulatory knowledge relates to how the host agency must meet procedural and quality requirements of the relevant jurisdiction(s) including public consultation rules and legal contestation options (Arnold and Marchildon 2018). Less formal, procedural knowledge covers how model applications are used to influence the policy decisions. This includes how results (and their uncertainty) can be communicated (Hare 2011), and how models can foster consensus building and legitimacy of science-based decisions (Voinov et al., 2010). Technical IT knowledge relates to the computer-human interface, and modelling knowledge consists of know-how on adequately representing the study system in the model, calibration, uncertainty estimation, numerical solvers, resolution and scaling aspects, and performance (Refsgaard and Henriksen 2004; Harmel et al., 2014).

These fields manifest themselves in further more generalized forms of knowledge: explicit knowledge that can easily be transferred from one human to another, and tacit knowledge that is often hard to communicate and expensive to transmit (Grant 1996). The terminology of general vs. specialized knowledge (Jensen and Heckling 1995) is somewhat analogous; organizations that handle specialized knowledge tend to compartmentalize decision processes and inadvertently decentralize decision making authority, with difficulties of transferring knowledge from one specialized department to another and a growing need for knowledge integration (Laniak et al., 2013).

A key aspect of model-focused knowledge management is continuous learning. New insights should build on and influence the body of existing knowledge within the whole agency. This need for continuity has deep ramifications for model management and knowledge infrastructure, partly in light of the short life cycles of computing systems that seldom out-live policy or management cycles (Marchildon et al., 2017). On the one hand, investment is needed to ensure that the knowledge encapsulated in a model is not lost as computing systems evolve. On the other hand, model management needs to ensure that existing models do not hold the organisation back. Models can potentially help organisations to be more adaptive and agile, by making tacit knowledge explicit, and hence supporting communication of new insights and reflection on the state of knowledge, leading to further improvements.

2.2. Model management across three embedded cycles

Model management operates across three embedded modelling cycles (Figure 1). This actor-centric
conceptualization is developed along the “regular” modelling steps (e.g. Jakeman 2006), by closely examining the actors which are involved at each level of a modelling process, what knowledge each actor brings to the process, and what types of decisions are expected (Arnold 2016). A core implication of understanding a modelling process as embedded cycles is that each policy cycle may require several reconceptualization cycles, and yet many more technical cycles. From a budgetary perspective, cost savings in executing one technical cycle (e.g. with automation) greatly reduces overall modelling costs. From an organizational perspective, it more clearly defines what type of decisions are expected, when and by whom.

The *technical modelling cycle* handles the traditional technical model set-up, the implementation of changes to the model, the re-running and re-calibration of models up to the creation of updated results, performance and quantified uncertainties. This technical cycle should embed all relevant IT and technical modelling knowledge. Typically, the technical cycle is performed by modellers and system scientists, with support from IT specialists. Any specific model application draws on the scientific knowledge available at that point in time.

The *conceptual learning cycle* handles learning about the real-world study system. This includes: the analysis and interpretation of knowledge about the system using data, models and local information; change scenarios that are to be evaluated with the model application; and changes to the assumptions and information utilized to simulate the system. Typically, conceptual modelling is done in stakeholder and expert groups supported by modellers (Voinov et al., 2016).

The *policy and management cycle* oversees the definition of a problem and a management goal. This includes delineating a system to be managed and the knowledge needs perceived as relevant, finding strategies to monitor the study system, assessing the system’s behavior with data and models, interpreting assessment results and building consensus around their implications, identifying policies and potential actions to achieve the management goal, making value judgement in assigning priority, implementation, and impact monitoring. Typically, people involved are managers or policy makers with limited technical or modelling knowledge (or interest). However, they are concerned about regulatory requirements, achieving policy goals, and budget allocation. In this context, modeling supports the policy and management cycle in framing and defining management problems, and prioritizing management options using “the best science available”.

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These three cycles are nested: the policy/management cycle defines the range of policy options that need to be assessed and the system boundaries. Any change to the conceptual understanding of a system may require iterating the technical cycle: re-calibrating and re-evaluating the model application. These additional technical cycles require financing and may stall the conceptual learning process. Conversely, limitations or new insights arising in the inner cycles inform higher level cycles and lead to changes in the system boundaries, system conceptualisation and decision options. At all times, participants in each cycle need be aware of their respective role in the decision process, and delegate value judgements to the appropriate and legitimate level of the hierarchy.

Knowledge requirements and information processing capabilities can vary significantly between participants across these three cycles. A particular challenge stems from the hierarchical nature of government agencies: knowledge about a problem is not always with the person who holds the power to make a value judgement. At the same time, modellers should support decision makers, without exerting (illegitimate) power through their own knowledge position. The aim of the technical modelling work is to reveal the relevance of the system interactions and associated uncertainty, based on the provided conceptual information and assumptions, and to translate results into a language that is accessible to stakeholders participating in the other cycles. It is the task of model managers to ensure that participants receive adequate information that aligns with their knowledge and their responsibilities, in a format that is tangible, within timelines and within budget.

In general, our understanding on how to manage modelling knowledge in real-world organizations is only emerging, in particular how to integrate modelling knowledge into the day-to-day operation beyond the narrow project focus. In most cases a structured approach to MNM is missing and environmental managers therefore fall back on short-term, ad-hoc solutions. For example, interviews with Ontario conservation authorities (Arnold and Marchildon 2018) indicated a focus on anticipated and immediate model outcomes, such as a consultancy report. But managers struggle to address longer-term tasks such as model maintenance, model updating and model reuse. Furthermore, little attention is given to incremental and continuous learning in relation to modelling, or identifying requirements for potential legal contestation of results by affected parties. In interviews, higher level management stated that explicit model management would create unreasonable overhead costs, and a typical response was that “our organization is not yet ready for model management” - in contradiction to Machildon et al., (2017)’s finding that “any agency that commissions numerical modelling studies does model management – either implicitly and unintentionally, or explicitly and with specific management goals”
Figure 1. Management of numerical models within three embedded modelling cycles (adapted from Arnold 2016): at a high level, the technical modelling cycle involves a number of tasks for specific environmental modelling site applications (model applications), which contribute certain functions to the organisation. Technical modelling tasks are interdependent with conceptual learning and policy & management activities. The model manager uses a variety of leverage points to ensure that the modelling tasks fulfil the required functions.

3. What does model management need to manage?

3.1. Modelling tasks of an organization

Our framework (Figure 1) considers that the model manager will need to organise the execution of five high-level modelling tasks: development of new model site applications, the operation and maintenance
of existing model applications, updating and sharing, and eventually archiving & decommissioning. This grouping pragmatically subdivides widely accepted modelling steps (e.g. Jakeman et al., 2006).

1. Development of new model applications

The development of a new model application is a resource-intensive process for the watershed agency or business. It requires a clear purpose, agreement on how project management can achieve the expected modelling outcomes, sufficient data, selection of an appropriate model code, and access to sufficient expertise and resources. Because budget and timing implications may be severe if these requirements are not met, Marchildon et al. (2017) recommend a scoping study (Chapter 5).

Obviously, before model results are published or used for decision making, adequate quality assurance procedures are required. As described by Hamilton et al., (2019), evaluation is a multi-faceted problem. Even in the case of establishing model credibility, there are a wide variety of approaches for the model manager to select (Guillaume et al., 2017). Performance assessment (Bennett et al., 2013, Harmel et al., 2014), uncertainty analysis and sensitivity analysis (Refsgaard et al., 2007; Matott et al., 2009) are key quantitative techniques, but require suitable expertise and can be computationally expensive, and therefore require appropriate computational infrastructure.

2. Operation and maintenance of existing model applications

Existing models may be employed for operational or strategic purposes, and often this is legally mandated. Operational purposes include real-time forecasting, e.g. for regulating dams or other flow infrastructure, or for predicting emergency situations. Existing models may also be used to assess flow characteristics after modifications of the flow regime, e.g. in response to a development application or for prioritizing engineering interventions. Some of these operational uses may require slight changes to the model, e.g. developing different water abstraction scenarios. In this case, model operators must ensure that the modifications are within the applicability of a given model specification and calibration (Schlesinger 1979).

As part of model maintenance, the model manager plays a key role in negotiating what work is needed to address uncertainty in fulfilment of the modeling purpose, how uncertainty is included in conceptual iterations and data updates, and whether new quality assurance methods may be required.
3. **Updating of existing model applications**

Updating of existing models may be required to improve their usability and transparency, or to incorporate new knowledge about the study system. Any aspect of the modelling process may require updating: the type and format of data; its storage; the version of the model code; refinement of the conceptualisation of the system; model scenarios that exceed the applicability of the original model, methods for evaluating model outputs; and/or any other aspects that are deemed relevant (Marchildon et al., 2017). Models may be updated in three ways: (1) *continuously on an opportunistic basis* whenever the need or opportunity arises; (2) *on a demand-driven basis*, triggered by changes of the modelled system (e.g. the installation of new well) or by software updates; and (3) *at a regular interval*, e.g. aligned with municipal planning reviews.

4. **Sharing of model applications or components of models**

Modelling agencies may opt to share complete model applications or components, which can be input data (e.g. an authoritative geological model), data processing tools, modules of model code or the entire code. Platforms that facilitate the sharing of model components are emerging in academia (HydroShare, CUAHSI, the Open Earth initiative), and in government agencies that encourage reuse of model code (e.g. USGS), and others that offer repositories of entire model applications. Examples of the last are repositories such as the Danish model database as described by Refsgaard et al., (2010) or the Netherlands Hydrological Instrument (De Lange et al., 2014).

Despite these initiatives, it remains a challenge for watershed agencies to decide how and when to share model applications and model components (Arnold & Marchildon 2018). Concerns include that users may take a model application out of context to undermine the legitimacy of an agency’s decision. This concern is greater if the agency is aware of methodological shortcomings, for example the agency cannot achieve state-of-the-art uncertainty assessment due to resource constraints. Furthermore, legal contestations in litigation bodies may imply significant costs exceeding the budget of watershed agencies, but that development corporations can easily afford (Arnold & Marchildon 2018). Promoting model transparency and clarifying liability will lead to more cost-effective approaches in relation to model contestation.

5. **Archiving model applications and decommissioning legacy code**

A final task of model managers is to design a long term storage of knowledge, including archiving files
and software code. Policy and management cycles are often long (10-15 years) and access to model applications and their embedded knowledge might not be continuously required. However, if a model application is revisited in the next policy/management cycle, a new application should first review all the knowledge that has been generated (Arnold & Marchildon 2018). Or alternatively, model results might have to be reproduced or reviewed for legal reasons. Guidelines exist on how to document model applications (e.g. ASTM D5718 - 13, https://www.astm.org/Standards/D5718.htm), but strategies regarding how to store model code that can be re-run and associated analysis tools are often lacking. For example, IT systems might have become outdated or software licenses have expired or are discontinued. Alternatively, model managers may decide to decommission legacy code and transfer embedded conceptual knowledge into modern software. There are no clear guidelines on when to maintain full model applications, or only components (e.g. data products), or how to effectively transfer knowledge from legacy applications into more modern ones. i.e. providing backward compatibility.

3.2. Functions of the modeling system

Modelling can fulfil a range of functions within a watershed agency. These functions are interdependent with all three embedded modelling cycles but particularly intertwined with the policy/management and conceptual learning cycles (Figure 1). Each function influences how modelling tasks are to be managed, in potentially subtle ways.

1. Modelling fulfills regulatory requirements or core organizational functions

Regulatory functions frame the modelling process within the watershed agency, and define the agency’s modelling tasks. Examples include delineation of vulnerable recharge areas, assessment of contamination risk, or real-time flood warning.

While budgets are mainly allocated to complete the regulatory requirements and core organizational functions, these expenditures could benefit many other functions within the organization. By realizing the broader benefits of modelling, model managers may enhance the workflow efficiency of an organization. An analogous example is how geospatial data management systems in watershed agencies were initially set up for one particular purpose, but have later found ubiquitous uses.
2. Modelling can help organize and share existing information

Beyond the original objective of a model applications, such application can help integrate and coherently contextualize large amounts of data that otherwise would not be accessible for communication and human interpretation. Model application may be used to test hypotheses on causalities within a system, in ways that expose inconsistencies in system information, identify knowledge gaps and false assumptions, and provide organizations with tools to enhance system knowledge.

The form of information to be provided by models may vary depending on the end-user. For example, model applications can be used to provide geospatial time series for locations where monitoring is not available. Such data can be used within the same agency or provided as a service to third parties. For example, global climate models provide weather forcing for future analysis in regional models (e.g. by the IPCC Climate Data Distribution Centre), and regional models like NOAA's Great Lakes Coastal Forecasting System (Alves et al., 2014) or regional weather models (Anderson et al., 2002) provide consistent boundary conditions for nested, smaller-scale applications. This cross-usage of model data is not only useful across scales, but also across departments in the same organization, e.g. surface runoff models provide infiltration data for groundwater models.

3. Modelling can influence the collection of new information

Model applications offer a formal mechanism to direct data collection/monitoring activities: they contextualize whatever knowledge and data exists and highlight gaps, inconsistencies, and the need to improve resolution. The data required for a model application for setup or for validation purposes can direct ongoing monitoring efforts. The same data may be useful for other purposes within the organisation. Especially if model applications are corroborated with quantitative uncertainty methods, modelling can help evaluate the value of information and prioritize future data collection efforts (e.g. identifying critical new monitoring sites and intervals).

4. Models support communication and policy insight

Model applications can provide visually appealing communication tools that make technical work accessible to the general public, for example by visualizing future system development paths and the
impacts of policy interventions.

If multiple intervention options are compared in a scenario analysis, then model applications are visual
decision tools that reveal policy impacts and quantify trade-offs (Lahtinen et al., 2017b), often across
multiple knowledge and departmental domains. Multi-criteria decision frameworks (Huang et al., 2011)
and other environmental decision support systems (Rizzoli et al., 1997, Argent et al, 2009) elucidate
how diverging value judgements of stakeholders can lead to divergent policy choices, and can support
negotiations and consensus building (Hämäläinen 2015).

4. Leverage points of the model manager

Model management supports organizations in fulfilling these modelling tasks and model functions.
Model management is thus regarded as a separate responsibility that frames and enables technical and
conceptual modelling tasks. This paper focuses on these higher-level responsibilities that define and
shape the organizational context in which modellers work. For example, the responsibility of model
managers is to ensure that modellers can do their job within budgetary and temporal constraints, in a
way that benefits the watershed organization as well as possible. Model management and technical
modelling responsibilities may be executed by the same staff or attributed to multiple individuals. But
what are the actual leverage points that model managers can apply?

By our definition of model management, the activities of a model manager address the governance of
model applications, operational support for modellers and model users, and administration of modelling
projects. In practice, this involves a combination of three practical leverage points (Table 1):
cyberinfrastructure, operational procedures & standards, and strategies to access knowledge and
skills. These three leverage points are interdependent, as will be elaborated further down.

1. Operational procedures and standards

Operational procedures and standards simplify the exchange of data and knowledge between
individuals, departments, and organizations. These procedures provide an array of diverse rules of
varying complexity, tackling different leverage points. Basic conventions on file naming and file
directory structures (Marchildon et al., 2017) and agreement on data exchange standards (e.g. the
NetCDF data format) can greatly simplify team work. Agreement on modelling steps (e.g. Jakeman et
al., 2006) and model reporting guidelines (e.g. ASTM 2013), and emerging agreement on metadata standards, modelling semantics and modelling ontologies (Villa et al., 2009) further streamline and organize the modelling process.

An example, well-developed, initiative is the Australian eWater, a not-for-profit entity that provides “capacity building, modelling tools, technical support services and a community of practice to support integrated water resource management, and water management governance” (https://ewater.org.au/about-us/, accessed April 28th, 2019). eWater offers several cyberinfrastructure products like SOURCE, an integrated water resource management modelling tool, and TIME, a workflow tool for creating, testing and delivering environmental simulation models. eWater also provides guidelines and procedures for the management of modelling projects, such as estimating resource needs, project duration, and knowledge requirements (e.g. Black et al., 2014). Other procedures can further govern the relation between agencies and their service clients, e.g. templates for service contracts for modelling consultants, or checklists for deliverables (Marchildon et al., 2017). At the methodological level, guidelines may specify generic criteria for selecting model code (e.g. Boorman et al., 2009 or Jenkinson 2012), choosing scientific methods, and/or even prescribe decision trees for which model codes to use.

2. Strategies to access knowledge and skills

Strategies to access knowledge include the training of existing staff, hiring of new staff, contracts with service providers, and a multitude of collaborative arrangements (Arnold 2013). For example, Ontario’s Oak Ridges Moraine Coalition is a not-for-profit collaboration operated by multiple local watershed agencies. The coalition shares resources to hire a designated model custodian (Marchildon et al., 2017). Most small agencies simply opt for hiring a modelling consultant, which is least disruptive to the public agency (Arnold & Marchildon 2018). Strategies around human resource and temporal commitments vary. These strategies have implications for how knowledge can be accessed, turnaround times, risk of losing access to some forms of knowledge, lock-in situations and other dependencies on a consultant, and difficulties to transfer tacit knowledge between agencies. Likely, there are a large range of approaches for dealing with these issues that might require further investigation.

3. Cyberinfrastructure

Adapting the definition of Beck et al., (2009), cyberinfrastructure is an integrated workflow
management system for automated collection, storage, retrieval, and analysis of data, accessible by multiple parties. Cyberinfrastructure includes various processing and visualization tools for collaboration with others and provides access to the monitoring information, as well as historical and other relevant data. Operational cyberinfrastructure can also include modules for decision-making and management. More generally, cyberinfrastructure entails the entirety of software tools that are utilized in sequence to create and analyze a model application, and communicate model results.

**Cyberinfrastructure tools** are offered in various forms and levels of sophistication and licensing approaches. Tools may offer uncertainty assessment modules for parameter variation experiments and parallelized computing (e.g. using PEST, Doherty et al., 2010). Other tools standardize model coupling (e.g. the OpenMI data exchange standard, Gregersen et al., 2007) or offer model sharing frameworks (e.g. HydroShare, OpenEarth), which provide access to several users for robustness analysis and quality control (Goodall et al., 2011). Other tools simplify data assimilation and processing (e.g. OpenDA, Ridler et al., 2014), data analysis and visualization (e.g. Lu & Arnold 2012). Parallelization cyberinfrastructure may also link into cloud-based computing, computer clusters, local multi-processors, or any combination of these. Tools can integrate with geospatial data products or web-based data and mapping platforms (e.g. Google Earth Engine).

Access to these software tools may be governed with open source, software licenses, service contracts, or any combination of these. For example, many open source engineering models (e.g. by USGS) are supported with commercial user interfaces that are embedded into larger software packages (e.g. the VisualModflow and AquaVeo products, or embedded modules such as the SWAT model code into QSWAT or ARCGIS). Some software providers offer proprietary tools for proprietary models (e.g. DHI products), while other providers like DeltaRes are moving toward a service model for fully open source cyberinfrastructure.

Only a few agencies utilize fully automated cyberinfrastructure systems that meet Beck’s stringent definition; these are typically dedicated Earth system modelling agencies, or well-resourced watershed agencies servicing large urban centres (Arnold & Marchildon 2018). Many smaller rural watershed agencies rely on the cyberinfrastructure of consultants, and only receive the modelling results, in the form of a report (Arnold & Marchildon 2018). In this case, reproducing model results requires access to the original consultant to access the relevant cyberinfrastructure tools. Other agencies obtained access to parts of the cyberinfrastructure: they receive executable model code and model input from

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consultants, but lack the ability to create control files, perform analysis on output files, or visualize results (Marchildon et al., 2017). In this situation, agencies are still restricted in quality assurance, reproducibility and the assessment of policy scenarios. Despite those limitations, Muste et al., (2013) conclude that “end-to-end engineering systems are poised to create a new paradigm for watershed science and management, enabling interdisciplinary teams to collaboratively understand and manage complex watershed issues to achieve long-term sustainability” (p. 572).

Investments in cyberinfrastructure for transparent & effective model management can build over time, and costs may be shared between several agencies and partners. The authors believe that it is feasible that even poorly resourced agencies utilize sophisticated cyberinfrastructure.

**Interdependence of leverage points**

The three leverage points of model managers are strongly interdependent. Workflow cyberinfrastructure increases the need for additional tacit technical knowledge for its setup and maintenance, while simultaneously decreasing the need for other computer skills (Arnold 2013) and enabling new strategies for accessing knowledge. A similar situation has occurred in the proliferation of central geospatial data management solutions that replaced ad-hoc data storage on individual desktops. Examples of tasks that can be easily automated (or otherwise remain bottlenecks) include, setting up and modifying control files, copying files, re-formatting and aggregating data, executing multi-run experiments, the aggregation and evaluation of outputs, and visualization (Lu and Arnold 2012). Likewise, operational guidelines and standards also foster transferability of knowledge while imposing an additional layer of technical expertise on an organization. Especially if cyberinfrastructure is shared with partners or service providers, agreement on clear data exchange standards and well-defined workflow interfaces/protocols can save considerable time and money (Whiteman et al., 2012, p. 28). Due to such interdependencies, model managers must carefully choose leverage points that optimize the utility of modeling within an agency’s budget and regulatory constraints, taking into account funding cycles, staff turnover, and technological decrepitude of aging IT systems.
<table>
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<tr>
<th>Cyberinfrastructure</th>
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<th>Knowledge &amp; skills and capacity</th>
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<tr>
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<td>3. Modelling software</td>
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<td>· Code &amp; licenses</td>
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<td>· Model execution &amp; calibration</td>
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<td>· Uncertainty &amp; sensitivity analysis</td>
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<td>· Output evaluation &amp; reporting</td>
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Table 1: Three leverage points how model managers can enhance knowledge infrastructure for numerical modelling
6. Examples of management of numerical models

Research on model management is still at an early stage. To highlight lessons that might be learnt and ideas needing further testing, we briefly review model management in a few fields of practice. In particular, we highlight how organizations implement cyber infrastructure and knowledge management in different organizational contexts and hierarchies.

Operations Research

Operations Research has a long history of using model-based techniques for operational and strategic decision making, and associated experience in managing modelling processes. A considerable interest has emerged in recent years in the management of behavioral factors in order to succeed in model-based problem solving (Hämäläinen et al., 2013). Given that the main currency of modelling is knowledge, it is important to acknowledge the role of people as sources of knowledge, knowledge processors, and as communicators of knowledge. As humans, modelers and users of models are fallible, can be biased, react to social pressures, and may sometimes act in self-interest rather than respecting their role as part of a team or an organization (Lahtinen et al., 2017a). In model management, the Behavioural Operations Research perspective suggests to recurrently ask questions such as “how expert and stakeholder opinions ought to be collected”, “how to train people to acknowledge their biases and learn to cope with them”, “how to facilitate and foster productive group dynamics and social interaction”, and “how results from models ought to be communicated so that stakeholders interpret them correctly.”

The development of model management practices, processes, systems and culture is a social process, which may lead to unwanted, inferior situations. Lahtinen et al., (2017a) identified reasons for getting stuck on an undesirable path in a modeling processes: lack of critical evaluation of strategic path choices, lack of resources preventing changing the path, preferences evolving to align with the path, hidden motives to stick with the path, sunk cost fallacy, and emergence of lock-in due to the structure and dynamics of a system. In model management, awareness of these drivers helps devise means to tackle their harmful effects. One remedy is a reflective attitude, whereby prevailing practices and new alternatives are seriously questioned and mistakes are acknowledged and corrected. An atmosphere of trust is an important contributor to the emergence of such attitude on a group level (Gregory et al.,
Furthermore, a vast amount of research points to the importance of adaptive processes. Practical means to increase adaptiveness include (peer) reviews, prototyping, and retaining some development funds rather than fully allocating them front (Lahtinen et al., 2017a).

**Earth Systems modelling agencies**

The most evolved model management exists in the developed hierarchical bureaucracies of Earth System Modelling agencies. These include meteorological and oceanographic services and climate change institutes. These agencies generally operate one or a few models of high complexity with significant runtime requirements, and rely on an organizational structure with designated departments to perform all tasks proven relevant during decades of operation. The organizational chart of such agencies clearly identifies fields of knowledge required for complex model workflows: the system knowledge of sub disciplines, data management, user support, IT support, monitoring network support, monitoring technologies, remote sensing, data assimilation, data quality control and verification, development of user interfaces and software, model development, regional and local representation, communication, research, and client services. With ample permanent staff, these agencies hold massive tacit knowledge in-house and are able to operate custom-tailored workflow management systems. Many workflow technologies used in these centres are freely available and well documented, e.g. in the series “Earth System Modelling - Vol 1-6” (Puri et al., 2013, ISBN 978-3-642-40940-0). The immense staffing costs of Earth System agencies are only justifiable because their work benefits entire countries. It is important to avoid holding up such cyberinfrastructure and governance structures as best practice or ideal - agencies need to adopt approaches that suit their particular circumstances and needs.

**Hydro-meteorological real-time forecasting and other research initiatives**

Hydro-meteorological real-time forecasting systems automate the use of meteorological monitoring data to forecast hydrological behavior, e.g. for the operation of dams or for emergency preparedness. Overall, publications and scientific workflow tools reflect those used by Earth System modelling agencies (e.g. Hally et al., 2015, Leonard and Duffy, 2016). Some of these systems also automate uncertainty analyses using multi-run experiments and provide tools for related output evaluation (Vivoni et al., 2011, Liu et al., 2012, Werner et al., 2013, Pagano et al., 2014).

Success stories published in the scientific literature often point out significant organizational difficulties in maintaining automated modelling workflows and the academic tendency of developing
YAMF (“yet another modeling framework”) that works as a pilot study but never matures into a reusable product (Rizzoli et al., 2008). Other challenges include timely and continued access to relevant knowledge, especially specialized technical IT expertise over longer time horizons, orchestrating large integrated projects (Arnold 2013), and overcoming the academic focus on publications (Hutton et al., 2016). Nevertheless, how operational forecasting models were established (e.g. Leonard & Duffy, 2016, Yu et al., 2017) can help guide development, and further research is recommended to mainstream these lessons.

Private engineering firms

Private engineering and for-profit consultants often specialize, such as in the set-up, operation and maintenance of hydrological models. Consultants may have economic incentives to keep the modelling process in-house, in order to gain an advantage over their competitors. Private consultants might also apply best business practices, including the assessment of workflow inefficiencies, with the goal of establishing structures that enable effective management.

The main success factor for engineering firms is effective knowledge management. The authors’ experience with such companies underlines a range of standards (from simple file structure over documentation standards, data formatting standards, to complex procedural guidelines), effective data sharing and analysis tools, and state-of-the-art data analysis and visualization software (e.g. Lu and Arnold, 2012). Companies can use mixed strategies of employment and outsourcing, combining hired staff for tasks that require frequent interactions, and service contracts for clearly delineated and well-confined standard tasks. Model management strategies reduce the dependence on individual staff through interfaces and documentation requirements. Companies nevertheless maintain key players who have understanding of relevant software steps, recognising that over-optimising for efficiency can have trade-offs in terms of robustness and resilience.

Academia-driven data and model hubs

Academia-driven data and model hubs offer platforms for sharing data, models and tools for collaboration in research and promote reproducibility in research. Examples include HydroShare, CUAHSI, GeoTrust, and the Open Earth initiative.

The lack of model management in public agencies is analogous to the reproducibility crisis in the academic fields of hydrology and geosciences. Hutton et al. (2016) describe this crisis as the inability
to reproduce published research findings created with computational methods. A response strategy of academics, funders and publishers is to conscientiously involve stakeholders throughout the modelling process (Pahl-Wostl 2002, Voinov et al., 2016); assign unique identifiers for data, code and authors (Hutton et al., 2016) and make data and software accessible in open repositories (Goodall et al, 2011); as well as adopting guidelines for scientific workflows and cyber infrastructure (Muste et al., 2013, Essawy et al., 2018). Ideally, modelers also recognize how their own behavior and cognitive biases (Hämäläinen et al., 2015, Lahtinen et al., 2017a) influence the outcomes of modeling studies; and scientists recognize procedural complexity of knowledge management especially when knowledge from multiple disciplines is integrated (Arnold 2013, Cobourn et al., 2018).

Recently, a broad initiative of geoscientists proposed the “Geoscience Paper of the Future” (GPF, Gil et al., 2016). They propose ways to ensure reproducibility of research through structured procedures for data and software accessibility and associated documentation, documentation of provenance and methods, and author identification. While these GPF guidelines facilitate reproducibility at dramatically reduced time and cost, they are not yet widely adopted by research journals, funders, and organizations (Yu et al., 2016).

The reproducibility crisis in science extends into decision making in natural resource management by public agencies. Firstly, numerous academics actively seek interaction with policy makers, e.g. by engaging with community stakeholders (e.g. Borowski and Hare 2007, Voinov et al., 2010). Secondly, researchers generally formulate their findings in a language of policy relevance, e.g. by recommending actions to policy makers that are amplified by popular media. Thirdly, public agencies actively draw on modelling methods developed in academia for making governance decisions, e.g. in the form of flood risk assessment, land use planning, drinking water protection, or more complex and inter-related goals. Decision making based on model results that are neither reproducible nor fully transparent poses a new technical barrier to participatory governance because power is shifted from local policy makers toward modelling professionals. Improvement in model management in public agencies therefore has the potential to improve reproducibility, avoiding broader implications for the legitimacy of democratic decision processes.
National-scale authoritative models

National water budget modelling initiatives face unique challenges in providing access to both model outputs and model data. Three national initiatives offer insights into the challenges and strategies when establishing nationwide hydrological models: the Netherlands Hydrological Instrument (de Lange et al., 2014), the Denmark Model (Højberg et al., 2013), and the UK National Groundwater Model (Shepley et al., 2012).

The three countries vary significantly in how the national models and the model databases were set up.

- In Denmark, this process was spearheaded by the Geological Survey (GEUS) that also hosts the Jupiter well database and now the Danish model database (Højberg et al., 2013). With a budget of approx. 200 Million Euros (personal communication, GEUS), GEUS orchestrated monitoring efforts and model updates with regional authorities and consultants and developed one central national database and model repository.

- The Netherlands Hydrological Instrument (NHI) evolved from ongoing modelling efforts at regional and national level. The NHI was set up with a budget of 1 Million Euros per year, contributed by water authorities and operators and supported by many academic organizations (de Lange et al., 2014). Partners are responsible for ongoing monitoring efforts and for maintaining distributed databases, and partners also contributed significant time from highly trained staff, in addition to NHI’s moderate core budget.

- In response to the EU’s water framework directive, the UK also established a National Groundwater Model (Hughes et al., 2012, Shepley et al., 2012) that continues to be developed, e.g. by integrating a recharge component (Farrell et al., 2017).

If not without challenges and learning, these national efforts successfully establish authoritative large-scale model applications that are still operational today. The three nations took very different model management approaches, e.g. with respect to hierarchy and centralization, open source vs. licensing, model complexity, and collaboration arrangements. One striking difference between the national approaches is the level of centralization. In particular the Dutch NHI offers a small central support agency that facilitates an otherwise decentralised learning process, contrasted by the UK’s attempt to maintain regionality, and the more centralized Danish approach. These organizational approaches are reflected in design choices for cyber infrastructure and handling of intellectual property rights: The Danish prescribe standardized data formats that can be used by many licensed and open model codes and processing software, as well as documentation standards. The Dutch require open source for all...
model codes and processing tools, compared with even a lack of data standards in the UK. In an interview (personal communication, Arnold 2017), Dutch staff pointed out that strong modelling skills available at their regional authorities was a success factor in their distributed approach, while Danish staff reported that modelling skills in rural and urban authorities are very divergent. In all examples, adequate handling of user expectations and communication with stakeholders was a key success factor.

**Ontario’s drinking water protection program**

Unlike the national, centrally orchestrated modelling approaches, the Province of Ontario has a decentralised approach to protect drinking water sources. When the Drinking Water Source Protection (DWSP) program was implemented in 2008-2012, municipalities and local water authorities had to develop model-based delineation of vulnerable zones around municipal wells and surface water intakes, and develop numerical water budget models in regions that were potentially at risk. The DWSP program thus serves as a case study of how different agencies chose to implement numerical modelling. Much of Ontario’s environmental governance is implemented through regional conservation authorities (CAs) that “develop and deliver resource management programs that safeguard Ontario’s watersheds” (Website, Ontario 2019). Given a strong contrast in modelling capacities between rural and urban watershed agencies, different approaches were chosen to meet the central provincial requirements. Urban agencies tended to employ staff to write requests for proposals (RfPs) and consulting contracts, review and test deliverables, suggest improvements, and manage archiving. Rural agencies, without access to modelling capacity, typically rely on past templates for writing RfPs, define deliverables, and draft consulting contracts. Additionally, “review consultants” were hired to comment on deliverables.

Arnold and Marchildon (2018) interviewed management staff from several watershed management agencies that supervise modelling studies to assess model management practices and issues. Generally, model management remained implicit without explicit goals or considerations to the long-term utility of model-related knowledge infrastructure. Only one agency defined explicit goals and objectives for model management, after a contentious and high-profile application for a permit to abstract and sell groundwater triggered consolidation of models across multiple jurisdictions, and explicit efforts to streamline modeling workflows. All watershed managers indicated that good technical guidance on modelling studies was available and were confident in how these were used by engineering consultants. With infrequent need for modelling knowledge, rural agencies were in no position to maintain in-house modelling capacity (staff or a designated department). No standardized guidance was available on the
contracting process at the time of research, so CA staff relied on modifying historic consulting contracts. None of the interviewees stipulated standardized file formats for contract deliverables as part of RfPs or contracts. While many final modeling products were stamped by the engineering consultant, interviewees believed that liability for potential model errors remains shared between the agency and the consultant, but were mostly unaware of legal details. Ownership of “the models” remained with the agency as the client, but there was no clarity what “a model” really entails. In three cases, model code was not accessible by the watershed manager – either because licensing costs were prohibitive, or because the model application utilized an outdated or privately owned model code. One CA is contracting the United States Geological Survey and its IT partner to improve their model code. Rural interviewees indicated that they would welcome support for standardizing the contracting process, but lacked the resources to initiate this process themselves. Across all contracts, data processing routines remain privately owned by the consultant meaning results cannot be reproduced independently. A rural CA interviewee who relied on the consultant for model archiving commented that they were locked into working with that consultant. Another interviewee pointed out that a complete model application was lost when a consultant migrated to Australia.

A message of several rural executives is that “their organizations are not yet ready for model management”. These executives feared the sustained overhead costs of ambitious modelling cyber infrastructure and the requirement for specialized staff. Compared with the expected benefits from modelling, these costs were perceived as unjustifiable. Executives also pointed out that urban and academic initiatives were perceived as overly ambitious within rural realities in funding and access to knowledge, and that there is no model management strategy available that respects their rural context.

**Ontario’s Oak Ridges Moraine Groundwater Program (ORMGP)**

In awareness of these challenges, several local agencies in Ontario founded the Oak Ridges Moraine Groundwater Program (ORMGP). These partner agencies finance a shared staff person as “model custodian”, who can advise watershed managers, review RfPs and contracts, and test deliverables, and is also keeping archives of all models for future reuse. The ORMGP offers three main programs: (1) a centralized database of all geologic and water information that is “likely the most comprehensive, actively-managed water-related database in Canada” (ORMGP 2019a). (2) A three-dimensional hydrogeological interpretation including conceptual geologic and hydrogeological models, and (3) numerical flow modeling tools to help analyse the regional and local flow systems and to help make
flow predictions (ORMGP 2019b). With Provincial funding in 2015, the ORMGP elaborated *A Guide for Actively Managing Watershed-Scale Numerical Models in Ontario* (“The Guide”, Marchildon et al., 2017). This guide is targeted to water resource managers in partnering organizations, with feedback from academic, government and private sector stakeholders. The guide clarifies vocabulary, offers standard contract wording, and standardizes deliverables (file directories, naming conventions) that lower the knowledge barrier to understanding a consultant’s model application. The guide also clarifies the responsibilities of the model custodian. While interviewees felt that it was too early to evaluate the impacts of a model custodian and the Guide on the costs of future modelling efforts, consultants see the Guide as providing clarification on their role, especially in cases where government staff has limited modeling experience.

**Lessons from fields of practice**

While data management has become mainstream among public sector agencies, model management has not received the same attention. However, the examples show that in many cases a lot of thought has been put into how models are managed, yielding valuable insights and good practices (see Box 1). The case study in Ontario, in particular, demonstrates significant opportunities for improvement in MNM. However, there are no blueprint solutions that serve the needs of all agencies. Instead, agencies face diverse contexts and have vastly divergent capacities, which requires finding appropriate model management strategies.

Such a strategy should consider the frequency with which modelling-related knowledge and skill sets are needed, the agency’s long-term model-related expenditure, and the ability to reduce the costs of individual projects by investing in infrastructure. Some fields of practice suggest that in-house staff is reasonable. For smaller agencies, pooling resources and employing a “model custodian” may be the most feasible strategy, as done by the Oak Ridges Moraine Coalition. Still, the management side of numerical modeling needs sufficient rigor and needs to offer strategies that work for a broad range of organizational realities. The guidelines of the Oak Ridges Moraine Coalition lists (1) transparency and participation, (2) minimizing the cost of collaboration by reducing transaction costs, communication errors and costs, (3) legal defensibility, and (4) sharing, reuse, and replicability (Marchildon et al., 2017).
MNM may benefit from a shift from knowledge as intellectual property, toward the provision of knowledge as a service, as in the Dutch NHI. The examples also highlight the need for a balanced approach to centralization, standardization, and IT sophistication. Low-hanging fruits for central standardization may include data exchange formats (see UK case study), metadata standards, standard naming of file directory structures and model files, templates for service contracts, rules for long-term archiving of models. Other aspects should respect the local availability of resources (funding, knowledgeable staff), and more research is recommended on how to do so effectively. The Oak Ridges Moraine Groundwater Program, through shared model custodianship, exemplifies an approach that can bridge between the ambitious requirements of reproducibility and rural organizational realities.

Together, the lessons and the case study clearly demonstrate that better management of numerical models is feasible today, especially if compared with the success in geospatial data management. Yet, this would require organizations to establish explicit strategies on how they manage models, modelling knowledge, intellectual property and licensing agreements, contracting practices, and modelling data and code. Such model management strategy should provide the board of directors or other high-level governing bodies with information about how effectively models are managed, without requiring deep technical modelling knowledge. A model management strategy could provide managerial direction how staff can strategically build modelling capacity, infrastructure, and organizational practices, ultimately enhancing transparency and accountability to modelling processes in watershed agencies.

**Box 1 Lessons about model management from fields of practice**

- **Custom solutions** for modelling workflows are possible, but at a cost that requires significant funding and generally a large geographic scope that benefits, as exemplified by Earth System models.

- **Light-weighted scientific workflows** for reusability and collaboration exist, and can be utilized for hydrometeorological real-time forecasting. Yet, the diversity of tools still requires significant technical skill that is a high entry barrier.

- **Powerful workflow solutions** that combine organizational standards and procedures, as well as professional workflow tools offer cost-effective solutions for model implementation and knowledge management, as exemplified by commercial consulting firms.
● The use of **academic data and modelling portals** can significantly improve reproducibility and demonstrate how data and software repositories can be combined with well-documented guidelines and support services. Yet, without enforcement by journals and funders, these are seldom utilized.

● **Decentralized modelling programs**, which require similar modelling projects in multiple locations, could significantly reduce costs by standardizing methods, formats, and even contract relationships. Yet, rural and urban agencies can access vastly different resources, so blueprint solutions to model management are not recommendable.

● **National modelling initiatives** highlight critical factors such as standardization of data and information, access to knowledgeable staff, and different strategies to access to software, such as prescribing open source or providing a standardized data interface.

### 7. Conclusion

This article has provided a conceptualisation of model management and its scope, and described the rules and standards, software tools, and knowledge access and retention strategies around numerical model applications. We then canvas current practice in model management in several sectors in order to draw out some initial lessons and illustrate the need for further research. A core weakness of public agencies remains that model management is often not yet regarded as a distinct activity requiring explicit attention, even if agencies are facing the outcomes of unintentional (and often poor) model management.

Our analysis highlighted three leverage points for enhancing model management: ensuring adequate operational procedures and standards, appropriate cyberinfrastructure, and feasible strategies to access knowledge. Model management strategies can be seen as a combination of these leverage points that respects the capacity and resources of an agency, while supporting it in fulfilling its tasks. There is a need to recognize the differential needs, for example, between rural and urban areas, and develop tools and guidelines that support diverse ways to manage modelling in a way that empowers agencies in their efforts to manage watersheds, without overwhelming their capacity and without absorbing undue staff time and resources.
This article is intended to provide a starting point model management and enhance integration of modelling within watershed governance processes. We believe that improving MNM offers a great opportunity for increased efficiency of using public resources. Most watershed agencies have neither explicitly defined their modeling objectives for environmental governance and decision making, nor an explicit model management strategy. With increasing climate variability, both clear objectives and a clear strategy can greatly enhance an agency’s ability to utilize given resources strategically in ways that build resilience. We hope that the language and rationale offered in this article can support efforts to embrace explicit model management, for example by informing and structuring model management strategies of watershed organizations.

8. Addendum

Declarations of interest

None

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