

Institution: University of Liverpool		
Unit of Assessment: 11 (Computer Science and Informatics)		
Title of case study: nDrites: Enabling Laboratory Resource Connectivity		
Period when the underpinning research was undertaken: 2002 – 2016		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	Role(s) (e.g. job title):	Period(s) employed by submitting HEI:
Prof Frans Coenen	Senior Lecturer - Professor	1990 - present
Prof Katie Atkinson	Lecturer - Professor	2005 - present
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Prof Michael Wooldridge	Professor	1998 - 2013
Period when the claimed impact occurred: September 2014 – December 2020		
Is this case study continued from a case study submitted in 2014? No		
<p>1. Summary of the impact</p> <p>University of Liverpool researchers developed nDrites in collaboration with laboratory software company CSols Ltd. nDrites is a multi-agent software system that provides much-needed connectivity between laboratory resources (analytical instruments, robots, laboratory data systems, and laboratory applications). Key impacts include:</p> <ol style="list-style-type: none"> 1. A CSols-Liverpool collaboration facilitated new products and improved existing ones (worth £2,420,000 in sales), and started three subsidiary companies. 2. Lab instrument manufacturers (Teledyne CETAC, Sciex, Shimadzu) improved productivity and product integration. CETAC saved approximately \$1,500,000 in development costs. 3. High-profile end users (Johnson Matthey, Proctor & Gamble, Crown Packaging, ThermoFisher) improved productivity and enhanced quality control. 4. Five UK water companies, serving approximately 19,850,000 users, improved water sampling efficiency by 25%, with resultant benefits to water quality and the environment. 		
<p>2. Underpinning research</p> <p>The University of Liverpool has conducted research into multi-agent systems (MAS) since 1998. In a MAS, agents are independent and have only local knowledge, and the system is decentralised (no agent is solely in charge). The central motivation behind MAS research is that, rather than designing a single monolithic system, it can be beneficial to design systems that are comprised of many independent agents. Three fundamental issues in MAS research are 1) designing agents with appropriate roles, 2) enabling communication between these agents, and 3) ensuring that the system is robust with respect to the failures of single agents [3.1].</p> <p>The unit addressed the problem of enabling communication in MAS (issue 2) by investigating ontology-based approaches and extensions of the Contract Net Protocol (a classic MAS protocol that was developed in the 1980s) [3.2, 3.3]. In the ontological approach, the agents use a shared ontology that makes the communication rules explicit, machine readable, and sharable. This allows agents to agree on a workflow that specifies, for example, which task each agent will perform and when. In addition, the unit proposed a task allocation framework for different objectives – for example, minimising execution time vs. financial cost – that uses failure prediction and redundancy to build robust workflows in the sense of issue 3 [3.4].</p> <p>In 2013, laboratory software company CSols Ltd. approached the unit for assistance in addressing issues of connectivity between laboratory resources. The research output of this collaboration was the <i>Laboratory-Resource-Multi-Agent-System</i> (LR-MAS), a novel MAS that developed bespoke agent roles and utilised the unit's research to enable communication between agents and ensure robustness of workflows [3.5]. The agents within LR-MAS include system configuration agents, instrument monitoring agents, and analytical monitoring agents. The system configuration agents use the ontology-based approach to communication [3.2, 3.3]; their goal is to configure and connect lab resources with minimal assistance from laboratory personnel. In a separate piece of research with CSols, the unit implemented instrument failure prediction in LR-MAS [3.6]. This allows the instrument-monitoring agents to implement robust workflows based on instrument</p>		

failure prediction [3.4]. The analytical monitoring agents oversee experiments and either rectify any issues automatically or alert appropriate personnel.

In LR-MAS, laboratory resources themselves are not considered as agents. Instead, every lab resource is augmented with a software wrapper, called an nDrite, that allows the LR-MAS to receive data from and exert control over the resource. nDrites use a declarative approach to facilitate communication between agents and lab resources [3.5].

As in the title of [3.5], the term nDrite – while technically only one specific part of the overall LR-MAS system – has been used both in the literature and by CSols to refer to the overall multi-agent system. In Section 4, the term nDrite is used in this wider sense.

The collaboration between CSols and the unit was funded by two Innovate UK KTP projects.

3. References to the research

[3.1] Wooldridge, M.J. (2002). *An Introduction to Multi-agent Systems*, John Wiley & Sons. ISBN-13: 978-0471496915

[3.2] Tamma, V.A.M, Phelps, S., Dickinson, I., and Wooldridge, M.J. (2005). "Ontologies for supporting negotiation in e-Commerce." *Engineering Applications of Artificial Intelligence*, 18 (2): 223-236. DOI: 10.1016/j.engappai.2004.11.011

[3.3] Paurobally, S., Tamma, V.A.M, and Wooldridge, M.J. (2007). "A Framework for Web Service Negotiation." *ACM Transactions on Autonomous and Adaptive Systems* 2 (4): 14.1-14.23. DOI: 10.1145/1293731.1293734

[3.4] Stein, S., Payne, T., and Jennings, N. (2011). "Robust Execution of Service Workflows using Redundancy and Advance Reservations." *IEEE Transactions on Services Computing* 4 (3): 125-139, 2012. DOI: 10.1109/TSC.2010.47

[3.5] Atkinson, K., Coenen, F., Goddard, P., Payne, T., and Riley, L. (2016). "nDrites: Enabling Laboratory Resource Multi-Agent Systems." In Baldoni, M., Muller, J.P., Nunes, I., Zalila-Wenkstern, R., eds., *Engineering Multi-Agent Systems, Revised, Selected, and Invited Papers from 4th International Workshop on Engineering Multi-Agent Systems (EMAS 2016)*, co-located with AAMAS 2016: 1-21. DOI: 10.1007/978-3-319-50983-9_1

[3.6] Coenen, F., Atkinson, K., Goddard, P., Payne, T. and Riley, L. (2015). "Data Stream Mining with Limited Validation Opportunity: Towards Instrument Failure Prediction." Proc. Data Warehousing and KDD (DaWaK 2015), Madria, E. and Hara, T., eds., *Big Data Analytics and Knowledge Discovery*, Springer LNCS: 283-295. DOI: 10.1007/978-3-319-22729-0_22

4. Details of the impact

Industrial laboratories depend on instruments, robots, and monitoring and data analytics applications. These resources are manufactured by a large range of companies, often using their own data formats and protocols. Thus, connectivity between instruments is often not available by default. However, without connectivity, one cannot automate the complex multi-instrument workflows that are required in a modern lab environment.

As a partial solution, limited connectivity has been achieved as follows: 1) Data from lab instruments is passed to a Laboratory Instrument Management Systems (LIMS), which stores and makes the data available to end users. 2) Direct connectivity between two instruments is created with bespoke interfaces. Both types of connectivity require expensive on-site visits by specialist engineers. As a result, very often full integration across the many instruments present in a typical laboratory has not been achieved, and laboratory workflows often relies on manual transfer of data and conversion of data formats, which is error prone, costly, and inefficient. Consequently, the lack of effective support for lab resource connectivity has become one of the main challenges facing the analytical instrumentation industry.

This challenge was a primary motivation behind the 40-member Allotrope Foundation standardisation initiative (founded 2012), which includes many of the largest instrument manufacturers worldwide. The Allotrope Foundation is pursuing a centralised (i.e., not multi-agent-based) standardisation approach to improve this situation. Despite an annual budget of \$2,500,000, the development of standards and their adoption in the sector has been slow (as

noted by Sciex, a world leader in mass spectrometry, who are both a member of the initiative and a beneficiary of the impact described in this case) [5.1].

CSols Ltd. has been working to improve lab resource connectivity since 1990. In 2015, CSols brought to market a novel, decentralised, approach jointly developed with the unit. Instead of relying on the success of a massive standardisation effort, connectivity is achieved through nDrites that receive data from and exert control over the resource, as explained in Section 2. The success of CSols' approach has been evidenced by the uptake of nDrite-enabled LabApps (CSols' term for laboratory software applications) by laboratory resource users. According to CSols' CEO, nDrites have *"transformed industrial processes [across] ... providers (the vendors) and users of analytical instruments... improv[ing] efficiency in a range of laboratory settings by reducing their costs, speeding up turnaround times, improving analytical quality and supporting regulatory compliance"* [5.2].

nDrites have significantly benefitted commerce and the economy in the UK and globally by impacting upon CSols and improving productivity across the analytical instrumentation industry. Significant impacts include:

- 4.1** CSols' business was transformed through the collaboration with the unit.
- 4.2** Key lab instrument manufacturers improved product integration and reduced (i) development costs, (ii) time-to-market, and (iii) installation times.
- 4.3** Principal lab instrument users (i) improved work practices, (ii) reduced human error, and (iii) enhanced customer confidence.
- 4.4** Major UK water suppliers benefitted from improved sampling efficiency and new comprehensive audit trails with resulting benefits to water quality and the environment.

4.1 CSols Creates New Products and Improves Existing Products

According to the CSol's CEO, the unit's approach has transformed the performance of its business. nDrites *"significantly improved the performance of our existing LabApps"* and *"massively reduced the cost of producing LabApps"*. This new approach has allowed a major extension of CSols' own LIMS, called LabCache, which sits beneath most of their major products [5.2]. These products include AutoDil (for automatic dilution, see 4.2), and RemoteSampler and BactiAnalyst (products for sampling and analysing liquids in the field, see 4.4). The CEO emphasised that *"All of these initiatives would not have occurred without this KTP"* [5.2, 5.3]. By December 2020, CSols had sold nDrite licenses and nDrite-enabled LabApps worth £2,420,000. nDrites have driven CSols' expansion with the launch of three profitable group companies between 2015 and 2017 [5.2].

4.2 Manufacturers Reduce Costs and Time-to-Market through Connectivity and Automation

Instrument manufacturers have used nDrites to improve productivity, reduce development costs, and reduce time-to-market for new products.

Teledyne CETAC, a world leader in sampling equipment for elemental analysis, began integration of CSols' AutoDil software with their High-Performance Liquid Dilution System in 2015, marking the first use of an nDrite-enabled LabApp. It was launched in March 2017 at the Pittsburgh Conference on Analytical Chemistry and Applied Spectrometry, a major laboratory instrument conference [5.3]. CETAC's VP of Marketing and Technology explained that *"we don't just have a stop-go command [now], we actually have dilution commands or more intelligent feedback commands so that systems can actually react to the data that's being generated in a far more intelligent way... using nDrites allows us to capture as much value as possible... and to develop much more technically challenging products ... which otherwise we simply wouldn't be able to do."* nDrites obviate the need for conventional development processes that provide instrument connectivity, which *"typically require four to six months of software engineering time... at approximately [\$500,000]."* In 2017, CETAC estimated a \$1,500,000 saving in engineering time over two years by using nDrites in the *"development of truly intelligent communication protocols among laboratory equipment"* [5.4].

Sciex, discussed above, and Shimadzu (a major analytical instrument manufacturer, also a member of the Allotrope Foundation) have both significantly benefitted from nDrite-enabled connectivity and product integration. In 2017, Shimadzu adopted CSols' AutoDil software to provide unattended automatic dilution for a range of applications used in the environmental, chemical, and food industries [5.3, 5.2]. The Chief Software Architect at Sciex reported that nDrite technology *"plays a major role" in resolving the need for "a comprehensive solution in the facilitation of workflows between instrumentation and backend systems,"* which are traditionally impeded by *"various needs of interconnecting huge numbers of different instrument types and different software applications."* For their customers, nDrites offer *"a means to consistently process the data across all the different instruments... and it truly is a dream solution for them"* [5.1].

4.3 Instrument Users Benefit from Increased Efficiency and Improved Quality Control

The ability of nDrites to facilitate automation in analytical processes has benefitted major companies that use analytical instruments. Crown Packaging, the #2 global producer of beverage cans, used CSols' LabApps to provide bidirectional integration between instruments used for measuring levels of trace elements in beverage solutions after they have been used with new can coating formulas. This *"provides capability to automate what was a manually intensive operation processing hundreds of samples per day. Crown can now run the whole analysis unattended ... allowing results to be generated much more quickly."* Consequently, development of new coatings is accelerated with benefits to consumer safety, health, and the environment [5.2].

CSols also worked with Johnson Matthey, a FTSE 100 global science and chemicals company, to address long-term problems associated with chemical speciation. Johnson Matthey have integrated nDrites with their spectrometers and analysers to determine the levels of elemental oxidation states of precious metals in recycled mining waste slurries. These determinations are currently difficult to automate; however, nDrites have provided Johnson Matthey with the unique capability of routinely performing this analysis and subsequently accelerating research into recycling processes [5.2]. Proctor & Gamble, a world-leading consumer goods company, used nDrite-enabled systems to connect and control robots and instruments for the production quality control of biological washing powders [5.2].

4.4 Water Companies Cut Sampling Errors, Improving Quality and Consumer Confidence

Issues of pollution from agriculture, industry, and transport make it extremely challenging to achieve good water quality. A recent UK Environment Agency Report called upon water companies to double their efforts in reducing pollution incidents, to better understand the range of chemicals in sewerage systems, and to help rejuvenate the UK's water environment [5.5].

To meet these goals, effective and reliable water quality testing and control is crucial. Since 2016, five major UK water companies (Northern Ireland Water, Northumbrian Water, Severn Trent Water, Affinity Water, South East Water), serving approximately 19,850,000 UK residents, have adopted CSols' nDrite-enabled RemoteSampler; additionally, water company United Utilities (7,000,000 customers) has adopted CSols' nDrite-enabled AutoDil [5.2, 5.6]. We focus on the use of RemoteSampler. In contrast to existing paper-based systems, where data is collected in the field and later copied into a LIMS, RemoteSampler only requires data entry by the user in the field. This data is validated against pre-configured limits and checked for errors on entry. RemoteSampler has been commended for improving sampling efficiency and accuracy and has increased customer confidence.

Efficiency. The LIMS and Compliance Reporting Manager for Northern Ireland Water stated that nDrite technology allows the processing of 36 samples per hour, compared to 6 per hour under their previous manual approach [5.7]. An estimate of a typical use case in the UK water industry noted that RemoteSampler provides a 25% increase in effective sampling time, a 17% reduction in fleet mileage, and a <12 month return on investment [5.6].

Accuracy and Meeting Regulatory Targets. Northern Ireland Water estimated that prior to the integration of nDrites with RemoteSampler, as many as 5% of their transcriptions were inaccurate and needed to be repeated [5.7]. Northern Ireland Water note that the ability to produce *"full audit*

trails [ensured] full accountability and full visibility” and allowed them to “comprehensively demonstrate that we have sampled correctly to meet the requirements of the United Kingdom Accreditation Service, as well as the requirements of the Drinking Water Inspectorate and the Northern Ireland Environment Agency. Without their approval we cannot operate” [5.7]. Northumbrian Water have used RemoteSampler since 2015 and their Head of Laboratories and Sampling confirmed that it is used to take approximately 70,000 samples a year to meet regulatory requirements [5.8]. In the context of the Environment Agency’s call for water companies to improve wastewater processing, both Northern Ireland Water and Northumbrian Water note that RemoteSampler allows water companies to “*robustly defend where [their] results came from*” when in disputes with water treatment works [5.8].

Customer Confidence. Improved efficiency and consistency serve to enhance customer confidence. Northern Ireland Water state that by ending their previous reliance on paper and pen processes and “*showing that our samplers were monitored and accountable [meant that] they got better acceptance and reception from customers when taking samples. It really did do wonders for customer confidence*” [5.7]. Northumbrian Water have set targets to decrease bottled water consumption in their operating areas in the next five years; a goal which aligns perfectly with the Environment Agency’s agenda. Northumbrian Water’s Head of Laboratories and Sampling notes that the nDrite-enabled RemoteSampler is key to this: having a “*professional situation where people ... see the quality of the water being tested*” will “*encourage people to drink tap water and reduce the amount of bottled water that is drunk*” [5.8].

Helping Environment Agencies. nDrites have provided additional positive impacts for water quality and the environment. An nDrite-enabled project between CSols and the Environment Agency has developed *BactiAnalyst*, a system to test UK beach bathing waters for harmful bacteria. Liverpool’s impact on water quality extends beyond the UK. In November 2020, CSols won – in collaboration with ThermoFisher – a €200,000 contract with the Belgian Environmental Protection Agency. The nDrite-enabled RemoteSampler received a 100% effectiveness score, far surpassing products offered by competitors Siemens and LabWare [5.2].

5. Sources to corroborate the impact

[5.1] Transcript of an interview with Sciex (manufacturer using nDrite technology) Chief Software Architect, transcription (May 2020), indicating use of nDrites, benefits to customers.

[5.2] Testimonial from CSols Ltd. CEO (September 2020), indicating changes in industry, improvements to CSols’ product, LabCache, nDrite sales, CSols’ expansion, Shimadzu & AutoDil, Crown Packaging, Johnson Matthey, Proctor and Gamble, water companies using nDrites, Environment Agency/BactiAnalyst, ThermoFisher/Watergroep.

[5.3] KTP Joint Project Report (submitted to Innovate UK, September 2017), indicating 25% profit increase from improved operations, developments would not have occurred without research, AutoDil launch, Shimadzu.

[5.4] Transcript of an interview with Teledyne CETAC (manufacturer using nDrites) Vice President of Marketing and Technology (September 2017), indicating use of nDrites and cost savings.

[5.5] Environment Agency report, [The State of the Environment: Water Quality](#) (February 2018), indicating water value, water companies’ role.

[5.6] [RemoteSampler Product Webpage](#), indicating product features and benefits

[5.7] Transcript of an interview with Northern Ireland Water (end user of nDrite technology) Laboratory Data Management System & Compliance Reporting Manager (May 2020) indicating processing times, previous resampling rates, improved regulatory compliance, robust proof of compliance, customer confidence.

[5.8] Transcript of an interview with Northumbrian Water Group (end user of nDrite technology) Head of Laboratories and Sampling (September 2020), indicating regulatory compliance, robust proof of compliance, improved confidence in drinking tap water.