

BITS :: Call for Abstracts 2024 - Oral communication

<i>Type</i>	Oral communication
<i>Session</i>	Bioinformatics Core Facilities and Research Infrastructures
<i>Title</i>	DRMAAatic: dramatically improve your cluster potential
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<i>Motivation</i>	<p>Enabling external applications to access the computational resources of an internal cluster infrastructure presents a significant challenge, especially in terms of granting access to external users. This challenge demands a robust solution that can bridge the gap between internal clusters and external interfaces, facilitating efficient job management while maintaining robust security measures. Traditional HTTP calls are not well-suited for tasks that require prolonged computation or execution on computational clusters. Scientific computations, in particular in life science and bioinformatics, often demand significant computational resources and may need to be distributed across multiple nodes within a cluster. Demonstrating the need for streamlined job creation and execution within web-based environments, the web server issue of NAR (Nucleic Acids Research) reveals a prevalent trend in the field of bioinformatics. Many web servers are actively developing customized solutions to facilitate job creation. These solutions often involve either direct execution on the server, potentially burdening its resources, or the establishment of bespoke connections to internal clusters for task execution. This trend is evidenced by the substantial number of published articles in recent years: 89 in 2021, 102 in 2022, and 81 in 2023. These figures emphasize the ongoing pursuit of optimizing computational workflows within web-based platforms.</p>
<i>Methods</i>	<p>To address this need, we introduce DRMAAatic—a versatile framework designed to enable distributed job execution across diverse Distributed Resource Managers (DRMs), empowering organizations to effortlessly leverage their internal clusters for external applications. At its core, DRMAAatic follows job execution within DRMs through a structured architectural framework. Built upon Django REST and DRMAA APIs, it seamlessly integrates with diverse resource managers, offering flexibility in resource utilization. Tasks are predefined entities encapsulating execution parameters and configurations, ensuring uniformity and ease of use. Leveraging Django Object-relational mapping (ORM), the system efficiently manages job metadata, task specifications, and user data. The authentication protocol, tightly integrated with ORCID, provides secure access, while throttling mechanisms prevent resource abuse. The administration interface empowers administrators to configure tasks, manage users, and monitor job submissions, ensuring efficient system operation.</p>
<i>Results</i>	<p>DRMAAatic fills this gap by providing a versatile platform that integrates the power of the DRMAA, with the accessibility of REST APIs. DRMAAatic supports REST APIs for job submission, retrieval, and a comprehensive array of options comparable to those available when submitting jobs directly within the cluster. This approach offers researchers the flexibility to execute a wide range of computational tasks, tailored to their specific needs, all through simple HTTP calls. DRMAAatic has been successfully implemented in various web servers published in NAR, including RING, CAID Prediction Portal, and Protein Ensemble Database (PED).</p>
<i>Info</i>	-
<i>filename</i>	-
<i>Figure</i>	-
<i>Availability</i>	-
Dissemination Material	
<i>Social</i>	Twitter: @AlexanderMonzon @BioComputingUP
<i>Summary</i>	-
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