Chatbot Guided Domain-science Knowledge Discovery in a Science Gateway Application

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***Abstract*—Neuroscientists are increasingly relying on high performance/throughput computing resources for experimentation on voluminous data, analysis and visualization at multiple neural levels. Though current science gateways provide access to computing resources, datasets and tools specific to the disciplines, neuroscientists require guided knowledge discovery at various levels to accomplish their research/education tasks. The guidance can help them to navigate them through relevant publications, tools, topic associations and cloud platform options as they accomplish important research and education activities. To address this need and to spur research productivity and rapid learning platform development, we present "OnTimeRecommend", a novel recommender system that comprises of several integrated recommender modules through RESTful web services. We detail a neuroscience use case in a CyNeuro science gateway, and show how the OnTimeRecommend design can enable novice/expert user interfaces, as well as template-driven control of heterogeneous cloud resources.**

***Index Terms*—neuroscientists, science gateways, recommender system, ontimerecommend, chatbot guided user iterface, knowledge discovery**

I. Introduction

Research and training in neural science and engineering increasingly deals with diverse and voluminous multi-parameter data [1], posing unique challenges outlined in an NSF iNeuro report [2] as limited access to: multi-omics data archives [3], heterogeneous software [4] and computing resources (Neuroscience Gateway [5], Amazon Web Services (AWS)), and multi-site interdisciplinary expertise (e.g., engineering, biology and psychology). Existing distributed high-performance computing resources (HPC) and other cyber infrastructures (CI) enable access to analyze and visualize such data. However, to fully utilize their capabilities, neuroscientists (often with limited CI skills) are required to take valuable time away from the focus of knowledge discovery in neuroscience, to learn how to use such technology.

There is a consensus that neuroscience research is also hampered by limited exchange of ideas, sharing of data, and collaboration within the community. In addition to these challenges, other factors such as reproducibility, usability, automation, and distributed cognition [6] have been significant barriers for use of science gateways (SG) in computational neuroscience. Labs pursue their individual research independently, distribute their research via journal articles, and reinvent the computing pipelines used in their analysis [7] time and again. To reproduce experiments done in other labs, it is imperative to disseminate the exact code and procedure used during the experimentation. This can be challenging especially to share distributed data for different artifact types and locations.

Such practices often results in redundant analysis scripts from these independent labs, which are often difficult to reproduce, due to poor coding skills, lack of version control and manual implementation of certain tasks [8]. Moreover, additional data at all levels of neuroscience continues to accumulate at rapid rates and volumes [9] [10]. However, the community lacks effective CI tools to harness such data sets and to also foster effective interdisciplinary interactions to advance the 'team science' research needed in neuroscience, in a scalable, reproducible, sustainable, and efficient manner. Productivity is also influenced by automating the workflow templates of common tasks that are repetitive. Hence, the template composition should be customized based on users' domain knowledge and workflow needs.

In this paper, we address above needs and to spur research productivity and interdisciplinary collaborations within neuroscience (i.e., our target community). Specifically, we describe our "OnTimeRecommend", a novel recommender system that comprises of several integrated recommender modules through RESTful web services. OnTimeRecommend features a multi-layer recommender architecture to increase the effectiveness of novice/expert neuroscientists using CI resources in workflow management within next-generation science gateways, as well as template-driven control of heterogeneous cloud resources.

The recommender system requirements are motivated by science application drivers within a CyNeuro science gateway [11]. CyNeuro utilizes CI resources (e.g., Neuroscience Gateway, JetStream, XSEDE, AWS) in order to integrate data, tools for data analytics, computing, and visualization with cyber and software automation. OnTimeRecommend features aim to supplement science gateways such as e.g., CyNeuro with application-facing modules that include: (i) Domain-specific Topic Recommender, (ii) Publication Recommender, (iii) Jupyter Notebook Recommender, and (iv) Cloud solution Template Recommender. Throughout the workflow users interact with a context-aware chatbot that is embedded with OnTimeRecommend which provides guided user interface, step-by-step navigational support and generates distinct re-

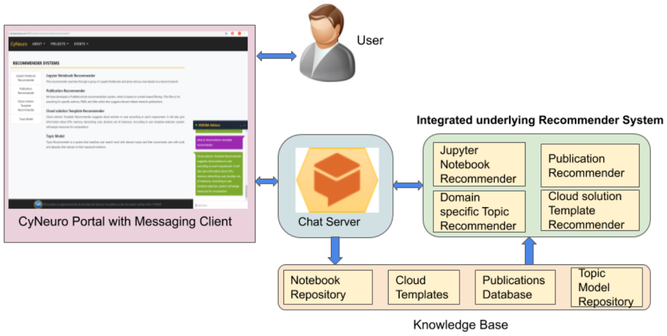

Fig. 1. Recommender system interacting with the CyNeuro portal through a conversational agent and chat server built using Dialogflow.

sponses for users based on user intent for guided educational and research purposes. The ultimate goal will be to ensure extensibility via RESTful APIs for custom configuration capabilities to support e.g., "BringYourApp", "BringYourOwnRecommender" as well as even "BringYourOwnHardware" within other science application community platforms using federated national CI resources.

The remainder of the paper is organized as follows: Section II presents the overview of our recommender system. Section III presents an exemplar neuroscience use case for the recommender system. Section IV concludes the paper.

II. System Overview and Background

Development of Science Gateway (SG) for federated national resources to improve accessibility in HPC/HTC resources at campus-level is an emerging concept in academia. At the U. of Missouri, a proof-of-concept for such a federated resource brokering has already been established to serve neuroscience educators and researchers at the university that benefit from a test deployment of the CIPRES workflow management software [12]. SG efforts are in collaboration with a large-scale national platform in the US i.e., NeuroScience Gateway (NSG) [13] that provides a variety of services for the users in terms of hardware and software.

One of our primary focus in this work relates to the educational and research aspects of using science gateways. Currently, there does not exist a science gateway system that is capable of easily and quickly allowing users to find necessary tools for their research, establish cloud infrastructure, search publications and execute code in a guided manner. To overcome such issues and facilitate multiple users to concurrently run simulations; find tools and datasets; and install hardware our work adopts the use of Jupyter Notebooks to run the code through Python and MATLAB kernels; topic model to find latest topics and trends in specific domain; and cloud templates to establish required infrastructure as shown in Fig. 1. Current practices require users to fully install all necessary technologies on their local laptops and need to understand or have expertise over the relevant configurations with little to no expert guidance. These specific activities pose a challenge for students beginning to learn neuroscience-related courses that require software to be installed and used.

Recommender systems with strong algorithms are at the core of today's most successful online companies such as Amazon, Google, Netflix and Spotify. With the growing amount of information on the internet and with a significant rise in the number of users, it is a difficult task for science gateways to search, map and provide the users with the relevant chunk of information according to the user's preferences and needs. In our OnTimeRecommend system, we have developed recommender modules with similar functionality in terms of providing recommendations of various resources to the target users based on their needs and preferences. By providing recommendations that suit users' requirement, our integrated recommender modules provide a personalized and expert advice across diverse computing platforms and data archives.

There are several examples of chatbot becoming user support agents in recent years [14]. In [15] and [16] authors presents a conversational recommender based on user functional requirements for suggesting the most appropriate smartphone. More recently, the bibliometric study on chatbots [17] reveals the scope of contributions in the state-of-art for chatbot applications in many domains with a high number of alternatives and thus, requiring automated user support.

In our previous work [14], we have proposed a conversational recommender that is used to provide a guided user interface and a chatbot functionality for neuroscience researchers and educators/students. The conversational agent design and integration with a CyNeuroscience gateway (built upon CIPRES) was described to support access of HPC resources for exemplar neuroscience research use cases. One of the main contributions of this work is a methodology for personalization that enables the chatbot to help users through customized recommendations. The users interact with a context-aware chatbot that is embedded within custom web-portals to obtain simulation tools/resources to accomplish their goals. The results are extended in this work for the neuroscience community to help researchers/educators to define new/diverse scientific workflows using local and remote HPC resources and foster collaborative efforts through their knowledge sharing via our recommender modules.

III. OnTimeRecommend Recommender System

"OnTimeRecommend" is a novel recommender system that comprises of several integrated recommender modules through RESTful web services as shown in Fig. 2. The OnTimeRecommend design enables novice/expert user interfaces within next-generation science gateways, as well as template-driven control of federated CI resources. The OnTimeRecommend features application-facing modules that include: (i) Domain-specific Topic Recommender, (ii) Publication Recommender, (iii) Jupyter Notebook Recommender, and (iv) Cloud solution Template Recommender.

Our recommender system is currently hosted on the AWS cloud, with our science gateway app (cyneuro.org) hosted on

Recommender Module	URL	HTTP Method	Parameters	Response	Description
Topic Recommender	/api/topics	POST	”text” : string	”topics”: [”id”:int, ”summary”:string,”tools”:string, ”datasets”:string, ...]	It receives query input of text and return json of relevant topics that contain topic id, summary, tools and datasets recommended for the topic
Publication Recommender	/articles/title	GET	”title” : string	”title”: [”_id”:string, ”ID”:int, ”Abstract”:string,”PMID”:string, ”Title”:string, ...]	It finds related content and necessary information based on the input title
Publication Recommender	/articles/authors	GET	”author” : string	”title”: [”_id”:string, ”ID”:int, ”Abstract”:string,”PMID”:string, ”Title”:string, ...]	It finds related content and necessary information based on the input author
Publication Recommender	/articles/pmid	GET	PMID : int	”title”: [”_id”:string, ”ID”:int, ”Abstract”:string,”PMID”:string, ”Title”:string, ...]	It finds related content and necessary information based on the input PMID
Jupyter Notebook Recommender	/api/jupyter	GET	keyword : string	”notebooks”: [”filename”:string, ”cell_no”:string, ...]	It searches for jupyter notebooks related to a given keyword
Cloud solution Template Recommender	/api/template	GET	application_type : string, site: string,memory:string,cpu:int, networking:string	”resources”: [”sgn”:string, ”memory”:string, cpu:int, networking:string, duration:int,cost:int]	Interface to receiving assistance regarding distributed CI resources assignment and expected cost for given hardware

TABLE I
DETAILED REST API FRAMEWORK FOR ALL RECOMMENDER MODULES IN ONTIMERECOMMEND

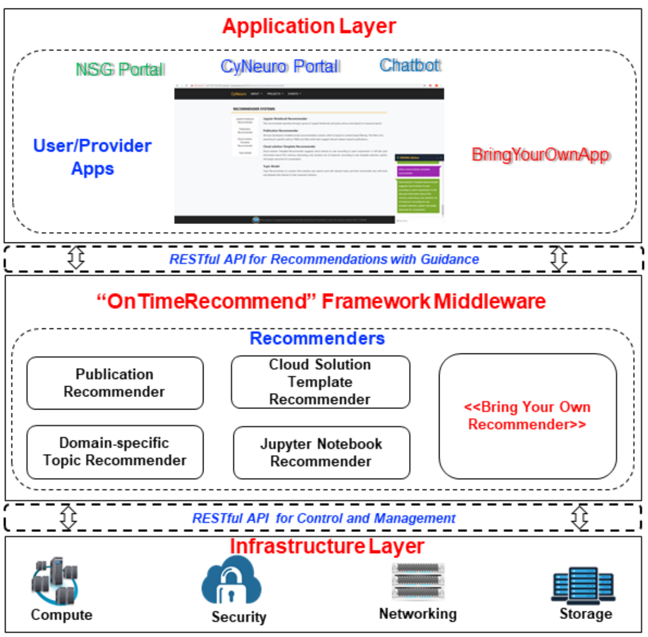

Fig. 2. Multi-layered OnTimeRecommend architecture with application-facing and infrastructure-facing RESTful APIs.

an EC2 instance that is connected to the recommender modules using REST API calls. While the storage need for our initial deployment is initial, the size of the instance grew from a micro to a medium instance as we began to run all necessary installations and configurations of the CyNeuro application. AWS CloudWatch, a dashboard that carefully monitors the health and performance of the instance is being used to monitor the application.

IV. NEUROSCIENCE TASK USE CASE FOR THE RECOMMENDER SYSTEM

Herein, we demonstrate an exemplar computational neuroscience use case that can benefit from our OnTimeRecommend system. For a neuroscience researcher who wants to build biophysical realistic single cell model, they typically have to perform extensive parameter searches to develop a model cell using biologically measured properties. We have two methods that can help researchers accomplish such a parameter search.

The first part is to simulate a single neuron model and quantify its electrophysiology properties given specific model parameters. Consider a Hodgkin-Huxley type of neuron model as an example, the parameters such as membrane capacitance, maximum conductance and reversal potentials of channels, etc., will determine the electrophysiological properties such as resting membrane potential, membrane time constant and rheobase current, etc. For example, the rheobase current is defined as the smallest injected step current of infinite duration which results in one action potential. The general protocol is to inject currents of various amplitudes, observe if any action potential is produced, and then further refine the injected current magnitude until the boundary between spiking and non-spiking behavior is identified. We use a Jupyter notebook recommender which suggests notebooks based on user query relevant to the functionality. User needs to input model parameters such as gbar_na, gbar_k, gbar_leak and a relevant notebook will returned with quantified properties after running simulations.

The second part is to predict the model parameters using a machine learning algorithm given desired electrophysiology properties. For example, let’s assume that the user provides FIR (frequency-current relationship) curves from experimental data and wants to know which set of model parameter such as gbar_na, gbar_k and gbar_leak can provide the particular FIR curve, In such a case, they can use an algorithm implemented in a Jupyter notebook which can be downloaded through guidance from the recommender system. The inputs include, but are not limited to, membrane time constant, membrane resistance, resting membrane potential, and sample points on the FIR curve. The algorithm uses a trained neural network to predict the model parameters. The notebook can help compare the FIR curve given by predicted model parameters and the target FIR curve in one plot. All other passive properties and spiking properties will be generated using the predicted parameters for validation.

For both the methods, once the researcher has notebooks, tools required to run the notebook would be easily comprehendible. The researcher can use topic model recommender to get the required tools from various latest publication repositories. The researcher may or may not have required infrastructure resources to run the notebook such as GPU. In this scenario the user can use the cloud template recommender to get an optimal template solution as per his preferred functional and nonfunctional requirements such as cost, performance and agility. The user can then deploy suggested cloud templates, install relevant tools and run notebooks over the resources to get relevant output corresponding to his input data. Based on the results, users can have their own evaluations and can further deep dive into their research with the feedback using the publication recommender. Thus, the integrated recommender system acting as a single source of knowledge discovery can cut down the mundane work and enhance user's research outcome and performance.

Considering the background of the neuroscience researchers, it could be intimidating to use neural networks or cloud templates. In such cases, our chatbot guidance can help in this scenario by providing the users with expert aid and navigational support whenever necessary. A novice user might need more assistance than an expert user which our chatbot takes into consideration in the dialog design which is used to respond to users based on their intent and proficiency profile [14]. Our integrated recommender system could thus potentially also save time and need for expertise on neural networks/cloud infrastructure usage, helping users to focus on their main research or education goals.

V. Conclusion

In this paper, we have proposed an integrated recommender system, the "OnTimeRecommend" that comprises of four recommender modules along with a guided user interface and a chatbot functionality for neuroscience researchers and educators/students. The OnTimeRecommend design and integration with a CyNeuro science gateway was described supporting an exemplar neuroscience research use case. The recommender modules can guide researchers and educators to discover relevant resources, enhance interdisciplinary knowledge sharing and train on Jupyter notebook enabled learning exercises. A cross-cutting multi-layer recommender architecture in OnTimeRecommend is designed to increase the effectiveness of novice/expert neuroscientists using CI resources in workflow management. Using text mining methods and topic modeling, the proposed recommender modules are aimed at fostering interdisciplinary collaborations around distributed databases, parallel and distributed computing resources for analysis and visualization of neuron simulations.

In future, our ongoing project activities seek to enable CI providers to integrate data analytic tools such that they improve efficiency of CyNeuro and other science gateway users in their research and education tasks.

Acknowledgment

This work is supported by the National Science Foundation under award number OAC-1730655. Any opinions, findings, and conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

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