GOMC Capstone

Software Requirements Specification

Version 1.1

October 7, 2017

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Revision History

Date	Version Number	Author	Version Notes
9/24/17	0.1	Caleb Latimer	● Implemented cover page ● Implemented revision history ● Implemented document approval ● Started Chapter 1
9/25/17	0.2	Caleb Latimer	● Implemented table of contents ● Intro ● Purpose & Scope
9/25/17	0.2	Muamer Besic	● Edited cover page ● Edited header/footer ● Added color ● Edited table of contents ● Formatted overall look
9/25/17	0.3	Ahmed Taher	● Added Downloads functional requirements 3.2.1 ● Added data flow diagram. ● Added a class diagram for the downloads model class
10/2/17	0.4	Caleb Latimer	● Implemented definitions table ● Implemented references and overview completing chapter 1
10/3/17	0.4	Ahmed Taher	● Added nonfunctional requirements ● Changed font size from 11 to 12 ● Organized downloads model and dfd into sections 4.2, 4.1

10/4/17	0.5	Ahmed Taher	● Added section 3.2.3 for login system
10/5/17	0.6	Caleb Latimer	● Reviewed and modified section 1.3 with new terms ● Refined all verbiage in the purpose, scope, definitions, and overview sections
10/5/17	0.6	Ahmed Taher	● Removed section 4.2 ● Worked on section 3.2.2 ● Worked on section 3.2.6 ● Worked on section 3.2.5 ● Worked on section 2.3.4
10/5/17	0.6	Muamer Besic	● Started Section 2 ● Completed section 2 description ● Completed section 2.2 ● Completed section 2.3 ● Changed body font to 12 TNR
10/6/17	0.7	Caleb Latimer	● Started and completed section 3.1 ● Added new requirements to section 3.2 for the UI ● Added references
10/6/17	0.8	Muamer Besic	● Completed section 2.6 ● Changed header colors to light blueish ● Completed section 2.1 ● Added screenshots of website prototype in appendix ● Went through whole document making sure format is same throughout
10/6/17	0.9	Ahmed Taher	● Added DFD’s level 0 and level 1 as well.

10/7/17	1.0	Caleb Latimer	● Added supporting documentation to the appendix section ● Linked references in 1.4 to various parts of the document ● Proofread, did some minor style tweaks and left comments in drive for feedback ● Redesigned the table in section 1.3 only displaying relevant terms first and the rest are now part of the appendix
10/8/17	1.1	Ahmed Taher	● Added section 2.4 and 2.5

Document Approval

The following Software Requirements Specification has been accepted and approved by the following:

Signature	Printed Name	Title	Date
	Ahmed Taher	Team Lead	
	Caleb Latimer	Lead UI Developer	
	Muamer Besic	Lead QA Developer	

	Azam Peyvandipour	Team TA	
	Younes Nejahi	Client	

Table of Contents

1. Introduction

The purpose of this document is to provide the reader with a thoroughly detailed explanation of the scope, design and implementation of the Wayne State GOMC Capstone Senior Design Project. Within this introductory segment an overview of all required knowledge will be provided. Following that, a detailed explanation of the functionality that this application will achieve, our design and build plan as well as an analysis of the different architecture involved and how they interplay. All acronyms, graphics and technical terms will be defined and established by a detailed explanation for the reader.

1.1 Purpose, Scope & Objective

The most fundamental goal of this project is to develop a dynamic modern website as a medium of presentation core for the research, development and new releases of the GOMC Project.

The GOMC Project is fully defined as the GPU Optimized Monte Carlo Method. It is a term that will be elaborated on largely in later sections of this document. But for the purposes of the introduction, we will generalize the definition as a simulation engine.

This engine is used to generate different classifications of molecular systems and using the Monte Carlo method - which we will elaborate on later - aims to optimize the system by making different changes to it. With each change the system's optimization strategy will refine itself by either accepting or rejecting the move. If the move is accepted it is implemented in the system and based on the resulting system another move is suggested. If it is rejected, the move is undone and removed the best-case scenario for this set of possible moves and another move is chosen to be suggested.

With the process of this simulation the structure is eventually optimized to sustainable VLE. Once the engine reaches this point the user is returned valuable data which can be used to optimize several factors about a chemical's development, production and storage. This kind of system is highly relevant to modern society as chemical manufacturing is a very in demand but also a very dangerous process. In terms of automating the production of the data as the result of experiments. Using the simulation as an alternative is not only faster, but it's safe for the environment and safe for all parties involved.

This project will encompass the full-scale design and implementation of a public website with the purpose of presenting a public face to the research and development of this engine by the Wayne State GOMC research group. The layout, color scheme, number of pages, functionality of pages and various other requirements will be laid out later in this document and be agreed on by the development team and client. Code, performance and style standards will be decided by the team with the client's approval. A key requirement of our software will require integration with the restful Github API v3 to dynamically produce announcements and update a downloads list with files released of code from the GOMC repository. This will automate the task of updating the pages between releases and aims to provide the fastest and most convenient experience for our users.

In addition to that, we will provide a form that allows a user to input some test parameters to generate the system and run the engine. The user will input data into the form and receive an input file for the application. The software will be modified by the Dev-team to run effectively with the input file as a source of valid data.

The GOMC Dev-team will also provide a doc-viewer which will allow the user to either download the official documentation or read in directly in the browser. The document viewer will allow for various forms of user interaction such as searching for a certain section or navigating quickly to other parts of the website. As the user manual is updated the doc viewer will be updated in direct correlation to that, so if the manual is updated the viewer will be updated as well.

Lastly, another area of improvement that we will implement is an admin dashboard. This will allow for the maintainers of the website to track meaningful data about the use of the website. It will also track data from github as a meaningful metric. All this data is valuable for continued improvement of the website overall.

These above four goals are the problems for our client that we will address as we design, develop and optimize our software to meet these needs, as well as the fundamental source of our functional and nonfunctional requirements that we will discuss fully in this document as we aim to develop a quality product.

1.2 Definitions, Acronyms and Abbreviations

All terms and definitions used during this project are defined in the Appendix. The below table contains a small subsection for some very specific terms that pop up a lot over the course of this document. For a fully comprehensive list please see the appendix section.

The headers indicate the overall group of these terms to provide an idea of the context that they may appear in. The table lists the term, acronym or abbreviation on the left with a simple explanation on the right. Some of the right cells of the table will include helpful links to provide further context of the term:

Term	Meaning
UI	User Interaction
UX	User Experience
VMD	Visual Molecular Dynamics
VLE	Saturated Vapor-Liquid Equilibria
MC	Markov Chain
Boltzmann	Boltzmann Sampling
Priority	Measurement of importance of a requirement 1 is most important (highest priority)
GOMC	GPU-Optimized Monte-Carlo simulation engine
GOMC Research	The team that our client is a part of
Repo	A folder stored in a remote location for development purposes
WFH	Work from home on a desktop environment
WFR	Work from remote on a laptop environment

CWFH	Checking in to work from home, seeing this in a commit message indicates that the developer is checking in their work to pull-latest on their desktop to continue work
CWFR	Checking in to work from remote, seeing this in a commit message indicates that the developer is only checking in to pull-latest on their laptop and continue work.
Pull-Latest	Pulling latest, grabbing latest or fetching latest all refer to grabbing the latest version of a branch on the repo
API	Application programming interface, in our case we will be referring to the github API v3
Standup	A daily report in our slack chat detailing what you did yesterday, what you are working on today and if you need support from anyone
UV	A demo to the client of some feature or design that they can give verbal feedback on. Also referred to as demos or client presentations
Beta	Our lower environment
Master	Our main environment
Downloads	A core feature of the downloads page using the github API
XML file	A core feature of taking form data, generating an xml file and sending that to an endpoint
Admin-Dash	A core feature of the admin dashboard

Doc-viewer	A core feature of converting and reading documents in html
P11 P12 and p2	Prototype 1-1, Prototype 1-2 and prototype 2
Site	When we say site, app or product we are talking about the whole summation of the deliverables
Ensemble	Structure and context of molecules
GOMC Dev-Team	The development team for this project also shortened to devs or dev-team
S1 - S7	Referring to screens 1- 7 of the of the current website
Distribution or dist/	A minified, uncommented version of a set of files. JavaScript files concatenated into a single file. Minimized for minimal bloat on client server and optimized for speed. This version of the code base runs in the production environment. It lives on our master branch in the repo and on our main server.
Source or src/	A development version of the code base. The exact opposite of the Distribution, lives on local. Changes to the code base are done to source first. Source is compiled, linted, validated, minified and tested before producing distribution. Source lives on our dev server and in our beta branch.
Master Server	Server supporting the website linked at the gomc.eng.wayne.edu space. Viewable by client and users.
Dev Server	Internal server for the team with code integrated from the beta branch. Can be found at ahtaher.net

Config Page	Also known as Config input page. This page is used for allowing the user to input config fields and then downloading the result as an XML file.

1.3 References

All external documents, papers and resources are outlined here:

1. Github, "Github API v3" https://developer.github.com/v3/
2. Amazon, "Amazon Relational Database Service (RD)" https://aws.amazon.com/rds/
3. Amazon, "Amazon Elastic Compute Cloud" https://aws.amazon.com/rds
4. Official GOMC Documentation http://gomc.eng.wayne.edu/GOMC_files/GOMC_Manual.pdf
5. GOMC github https://github.com/GOMC-WSU/GOMC
6. Code standards for C# https://docs.microsoft.com/en-us/dotnet/csharp/programming-guide/inside-a-program/coding-conventions
7. Bootstrap conventions http://bootstrapdocs.com/v3.0.3/docs/getting-started/
8. Materialize conventions http://materializecss.com/
9. jQuery conventions https://api.jquery.com/
10. Gulp JS https://gulpjs.com/
11. Unit testing C# https://docs.microsoft.com/en-us/dotnet/core/testing/unit-testing-with-mstest
12. QUnit http://api.qunitjs.com/
13. Github webhooks https://developer.github.com/webhooks/

1.4 Overview

The remainder of this document has 2 major sections. The next section will present a more detailed description of the system and all the required parts within. The third segment will detail the requirements needed for our application to be successful. Lastly, we have some diagrams and supporting files.

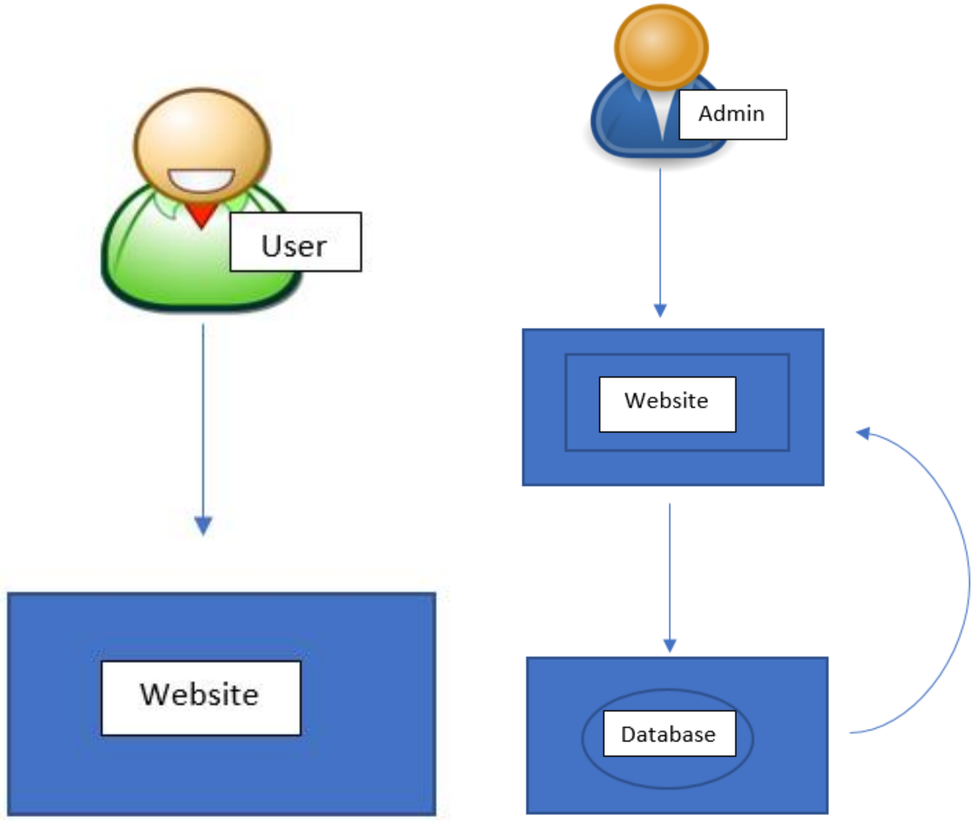
2. General Description

This section will give an overview of the whole website. The website will be explained in its framework to show how the website interacts with other systems as well as it will be introduced on its basic functionality. This section will also go over what types of users are prone to use this website and how different functionalities will be created to fulfill their needs. Lastly, the website's constraints and assumptions will be addressed.

2.1 Product Perspective

The GOMC Capstone project is a redesign and upgrade of an already existing website that is intended to be used on both computer and phone platforms. However, the website will be mainly navigated to by researchers using a computer rather than a smartphone. The reason for this is self-explanatory and it is because it is much easier for them to sit at a computer and do research rather than plug stuff in on their smartphone all day. The website will have a database for which the uses of it aren't 100% clear however, the main uses of the database would be used for storing the admin username and password, storing data about the forms submitted, and possibly even storing data about the downloads. For storing data about the downloads, we mean that it could be used to track who downloaded a file, from where, and how they intended to use it.

When it comes to the config form, it will not be storing any data in the database. What the config form will be doing is validations for the input fields in making sure the form is filled out correctly for example a field that is only supposed to have numbers entered, does not have any letters inputted. Below I have created a diagram illustrating the interactions between users and the website as well as admin and the website.



So, in the above illustration we see that normal users can go on the website directly without having to sign in however, it's a different story for admins. Admins will go on the website and will have to sign in to be classified as admin and receive admin permission with the website. Once they attempt to sign in, the username and password will be checked by sending it to the database and if the information entered is correct, it will come back by approving the login.

2.2 Product Functions

With the website created, researchers will be able to view several different forms of information. Below we have made a list which outlines different features on the website as well as a description of each one.

1. Menu Navigation bar
    - ❑ Home
    - ❑ Resources
    - ❑ Documentation
    - ❑ About

2. Github Releases
    - ❑ Fetches new releases from Github website
    - ❑ Allows user to download new release with just a click
    - ❑ Not required to be registered with website to be able to download releases

3. User Registration
    - ❑ Allows the user to register with the GOMC website
    - ❑ User will be informed about future releases/announcements
    - ❑ All information provided will not be publicly viewable

4. Links Available
    - ❑ Direct user to different sites such as:
        - ➔ GPU Research Center
        - ➔ Silicon Mechanics 3rd Annual Research Cluster Grant
        - ➔ National Science Foundation
        - ➔ Cornell University Library
    - ❑ GOMC Manual available that goes through all the small details
    - ❑ PDF links for different Monte Carlo simulations and developments
    - ❑ Download page links

5. Config Form
    - ❑ Allows researcher to input different data collected
    - ❑ Form is validated in each of its input fields
    - ❑ XML config input file will be able to be downloaded once form is filled out
    - ❑ Simulations are ran using the input file generated

6. Resources Available
    - ❑ Tutorials will be made available for those seeking to gain/refresh knowledge
    - ❑ Examples will be posted of how different things are done

2.3 User Characteristics

The GOMC Capstone project website is meant to be used by faculty, graduate/undergraduate students, and alumni in the computer science and chemistry fields. The website will mainly be used for research so each of the users will be visiting the site to either get new Github releases/downloads or fill out the config form to generate XML input files.

This project is meant to offer a more user-friendly dynamic website which offers users the ability to spend countless hours researching while having everything they need at their fingertips. The website will have a menu bar which includes easy-to-find pages making it easier for the user to be able to just look at the menu name and know that this is where they must go to find what they are looking for. Consequently, the config form will be created to make the lives of researchers easier by making the form simple to fill out each of the fields required without hesitating or not knowing what is asked. However, if the researcher does not know what is being required in a certain input field, they will be able to hover over the input field or in some other way perhaps click on a link, which will explain exactly what is being required in that field.

The administrators will be managing the overall website so there is no incorrect information within it as well as taking care of any occurring problems. They can change features as well as add any new features they might want in the future.

Users can use the website and all its features without having the ability to modify any parts of the website. Users can click on links, register, and fill out the input generator whenever they please to do so.

2.4 General Constraints

Users are required to have an internet connection. Since the project is a dynamic website, without an internet connection it is simply impossible to use the features of that website.

2.5 Assumptions and Dependencies

It is assumed that the user has access to a modern web browser capable of rendering HTML5. The website itself uses modern web development technologies which take advantage of HTML5.

As such, without a browser the content cannot be viewed by the user and without a modern browser the content may not be displayed correctly.

2.6 User Documentation

The primary goal of GOMC Capstone is to provide researchers with a website to continue their research work and findings. At the same time, the website will be created to be as simple to use and find things as it is convenient for its primary goal for researchers. However, users may still need some accommodating information about each input field when it comes to filling out the config form. The website will have features such as the GOMC manual, tutorials, examples, and a help option that will be provided for users to look at and ask any questions they want answered.

The about page will be a collection of the features listed above such as the GOMC manual, tutorials, and examples. The user can at any time navigate to the about page to look at helpful pieces of information that could be for example some formulas they are not sure of or what type of input the “Temperature” or “Pressure” fields in the config form require.

The user can look at the GOMC manual which goes in depth about the existing GOMC project and website. The tutorials and examples that will be provided will showcase different solutions for problems as well as how to go on to finding solutions for problems the user may be experiencing.

3. Specific Requirements

This section will outline the needs of the features that our application will support. This section will cover a high-level overview of the core requirement. The next will cover the external interfaces required for interaction with the application, then we will discuss the functional requirements and nonfunctional requirements providing full detail for what is needed for this to work. Lastly, we will discuss the design requirements and database structure before wrapping up and continuing into the next section of analysis models.

Our product will have a group of 7 core features each spanning their own list of requirements. All of them will have dependency on the first requirement which is of the highest priority for the dev-team, all requirements must be fully implemented, tested and approved by our client to ensure a fully functioning application both client side and admin side.

All 7 of our features are elaborated on at a high level in the below table and expanded on in extensive technical detail in the next subsection.

Feature	High-Level
Dynamic Website	A newly design and improved modern UI that is approved by our client
Automatic Downloads Page	The downloads page in the website must dynamically update its content as new versions of the software release
XML downloadable input file	The website must have the capability for users to input technical data and receive an XML download of their input that is well formed to run with the simulation engine
XML input file processing	The simulation engine must be modified to process and handle the XML input file format
Administrative Metadata collection	The simulation engine must send a phone-home package once it has been downloaded with administrative metadata
Document viewer	The website must have a document viewer that supports quick searches
Admin Dashboard	The website must present an admin page, once the admin is logged in they should have a dashboard of meaningful data

	to track usage reports

3.1 External Requirements

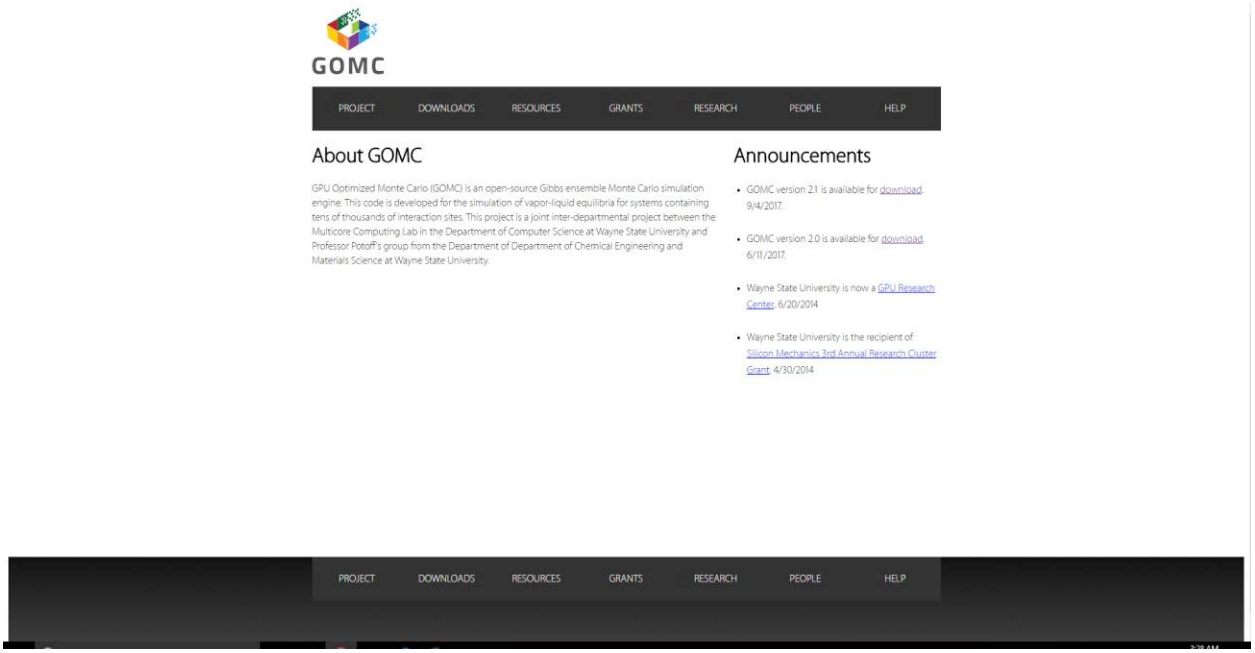
The purpose of this section is to in detail explain the required hardware, software and other factors that must be in play for optimal performance of the application.

3.1.1 UI

This segment will discuss UI requirements and expectations. The UI for our application consists of the website. The website will retain all its current data http://gomc.eng.wayne.edu/ [4]

Below are 7 images of the current website which will be referred to as S1-S7 respectively. **NOTE**: Images have been scaled to reflect full content without scrolling.

Project



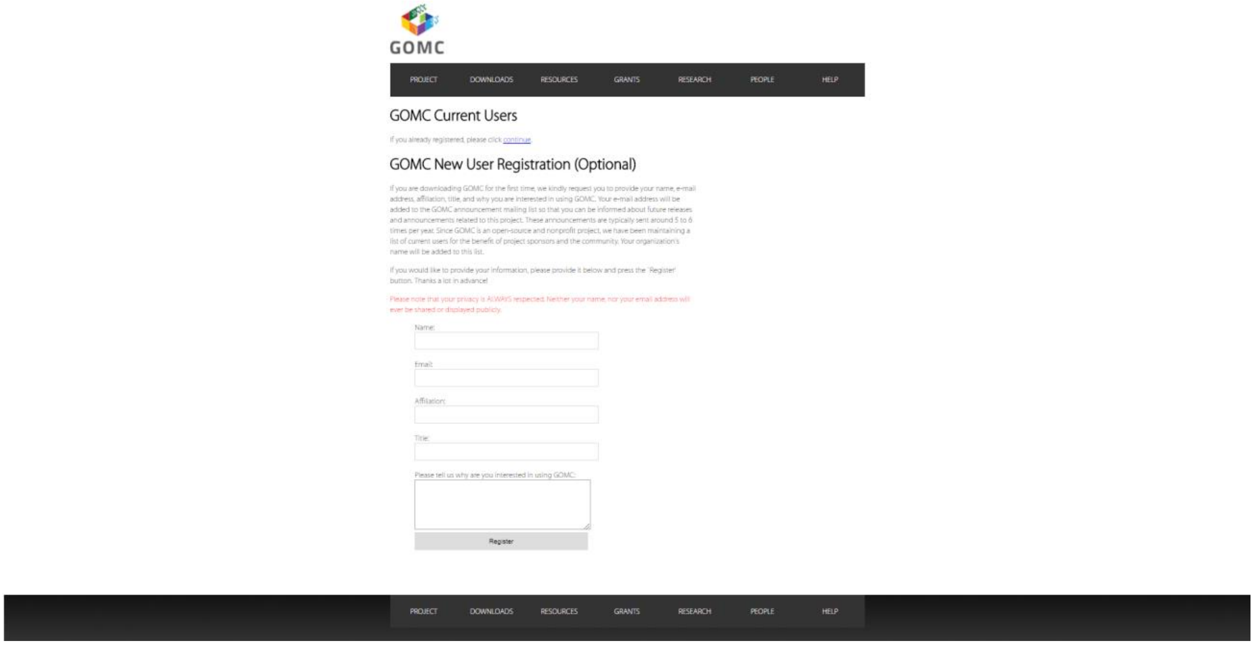
About GOMC

GPU Optimized Monte Carlo (GOMC) is an open-source Gibbs ensemble Monte Carlo simulation engine. This code is developed for the simulation of vapor-liquid equilibria for systems containing tens of thousands of interaction sites. This project is a joint inter-departmental project between the Multicore Computing Lab in the Department of Computer Science at Wayne State University and Professor Potoff's group from the Department of Department of Chemical Engineering and Materials Science at Wayne State University.

Announcements

- GOMC version 2.1 is available for download. 9/4/2017.
- GOMC version 2.0 is available for download. 6/11/2017.
- Wayne State University is now a GPU Research Center. 6/20/2014
- Wayne State University is the recipient of Silicon Mechanics 3rd Annual Research Cluster Grant. 4/30/2014

Downloads



GOMC Current Users

If you already registered, please click continue.

GOMC New User Registration (Optional)

If you are downloading GOMC for the first time, we kindly request you to provide your name, e-mail address, affiliation, title, and why you are interested in using GOMC. Your e-mail address will be added to the GOMC announcement mailing list so that you can be informed about future releases and announcements related to this project. These announcements are typically sent around 5 to 6 times per year. Since GOMC is an open-source and nonprofit project, we have been maintaining a list of current users for the benefit of project sponsors and the community. Your organization's name will be added to this list.

If you would like to provide your information, please provide it below and press the 'Register' button. Thanks a lot in advance!

Please note that your privacy is ALWAYS respected. Neither your name, nor your email address will ever be shared or displayed publicly.

Name:

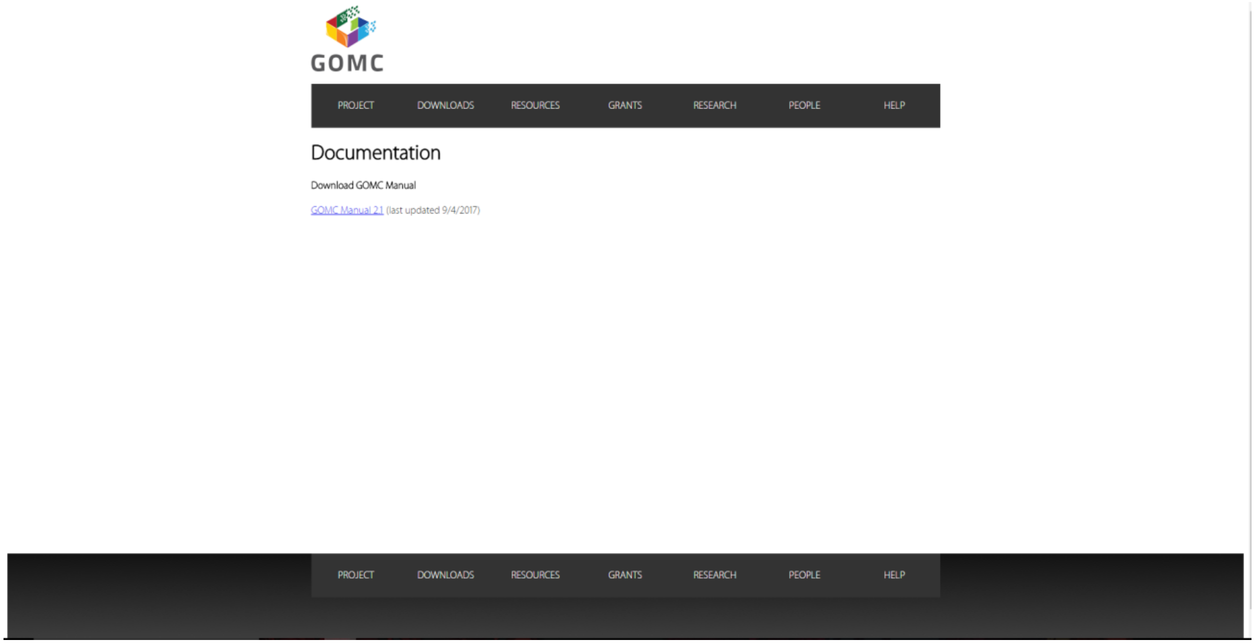
Email:

Affiliation:

Title:

Please tell us why are you interested in using GOMC:

Resources

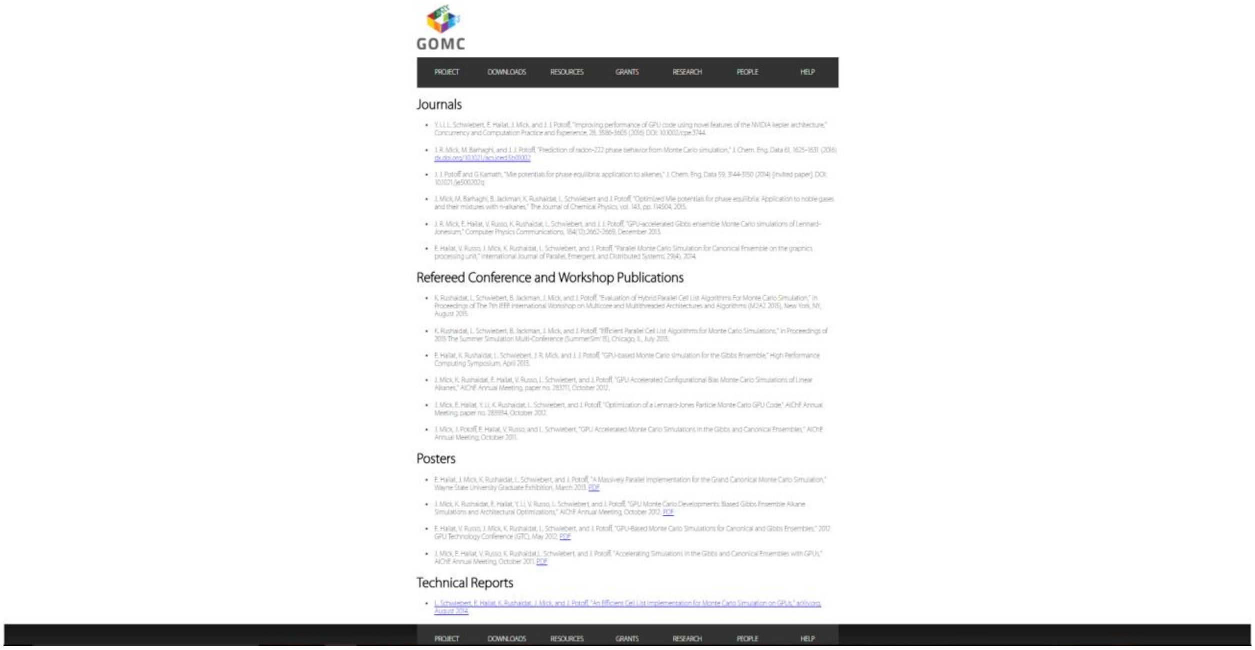


Documentation

Download GOMC Manual

GOMC Manual 2.1 (last updated 9/4/2017)

Research



Journals

- Y. Li, L. Schwiebert, E. Hailat, J. Mick, and J. J. Potoff, "Improving performance of GPU code using novel features of the NVIDIA kepler architecture," Concurrency and Computation Practice and Experience, 28, 3586-3605 (2016) DOI: 10.1002/cpe.3744.
- J. R. Mick, M. Barhaghi, and J. J. Potoff, "Prediction of radon-222 phase behavior from Monte Carlo simulation," J. Chem. Eng. Data 61, 1625-1631 (2016) dx.doi.org/10.1021/acs.jced.5b00002
- J. J. Potoff and G Kamath, "Mie potentials for phase equilibria: application to alkenes," J. Chem. Eng. Data 59, 3144-3150 (2014) [invited paper]. DOI: 10.1021/je500202q
- J. Mick, M. Barhaghi, B. Jackman, K. Rushaidat, L. Schwiebert and J. Potoff, "Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes," The Journal of Chemical Physics, vol. 143, pp. 114504, 2015.
- J. R. Mick, E. Hailat, V. Russo, K. Rushaidat, L. Schwiebert, and J. J. Potoff, "GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium," Computer Physics Communications, 184(12):2662-2669, December 2013.
- E. Hailat, V. Russo, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "Parallel Monte Carlo Simulation for Canonical Ensemble on the graphics processing unit," International Journal of Parallel, Emergent, and Distributed Systems, 29(4), 2014.

Refereed Conference and Workshop Publications

- K. Rushaidat, L. Schwiebert, B. Jackman, J. Mick, and J. Potoff, "Evaluation of Hybrid Parallel Cell List Algorithms For Monte Carlo Simulation," in Proceedings of The 7th IEEE International Workshop on Multicore and Multithreaded Architectures and Algorithms (M2A2 2015), New York, NY, August 2015.
- K. Rushaidat, L. Schwiebert, B. Jackman, J. Mick, and J. Potoff, "Efficient Parallel Cell List Algorithms for Monte Carlo Simulations," in Proceedings of 2015 The Summer Simulation Multi-Conference (SummerSim' 15), Chicago, IL, July 2015.
- E. Hailat, K. Rushaidat, L. Schwiebert, J. R. Mick, and J. J. Potoff, "GPU-based Monte Carlo simulation for the Gibbs Ensemble," High Performance Computing Symposium, April 2013.
- J. Mick, K. Rushaidat, E. Hailat, V. Russo, L. Schwiebert, and J. Potoff, "GPU Accelerated Configurational Bias Monte Carlo Simulations of Linear Alkanes," AIChE Annual Meeting, paper no. 283711, October 2012.
- J. Mick, E. Hailat, Y. Li, K. Rushaidat, L. Schwiebert, and J. Potoff, "Optimization of a Lennard-Jones Particle Monte Carlo GPU Code," AIChE Annual Meeting, paper no. 283934, October 2012.
- J. Mick, J. Potoff, E. Hailat, V. Russo, and L. Schwiebert, "GPU Accelerated Monte Carlo Simulations in the Gibbs and Canonical Ensembles," AIChE Annual Meeting, October 2011.

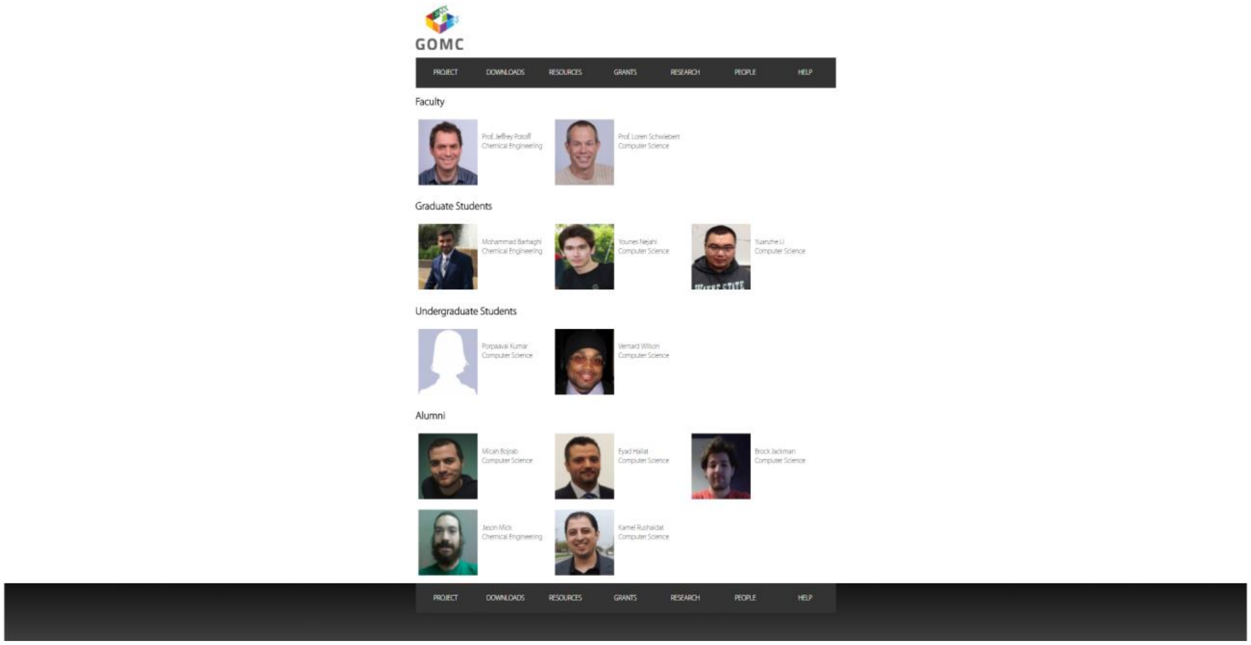
Posters

- E. Hailat, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "A Massively Parallel Implementation for the Grand Canonical Monte Carlo Simulation," Wayne State University Graduate Exhibition, March 2013. PDF
- J. Mick, K. Rushaidat, E. Hailat, Y. Li, V. Russo, L. Schwiebert, and J. Potoff, "GPU Monte Carlo Developments: Biased Gibbs Ensemble Alkane Simulations and Architectural Optimizations," AIChE Annual Meeting, October 2012. PDF
- E. Hailat, V. Russo, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "GPU-Based Monte Carlo Simulations for Canonical and Gibbs Ensembles," 2012 GPU Technology Conference (GTC), May 2012. PDF
- J. Mick, E. Hailat, V. Russo, K. Rushaidat, L. Schwiebert, and J. Potoff, "Accelerating Simulations in the Gibbs and Canonical Ensembles with GPUs," AIChE Annual Meeting, October 2011. PDF

Technical Reports

- L. Schwiebert, E. Hailat, K. Rushaidat, J. Mick, and J. Potoff, "An Efficient Cell List Implementation for Monte Carlo Simulation on GPUs," arXiv.org, August 2014.

People



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Younes Nejahi
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Computer Science

Alumni

Mican Bojrab
Computer Science

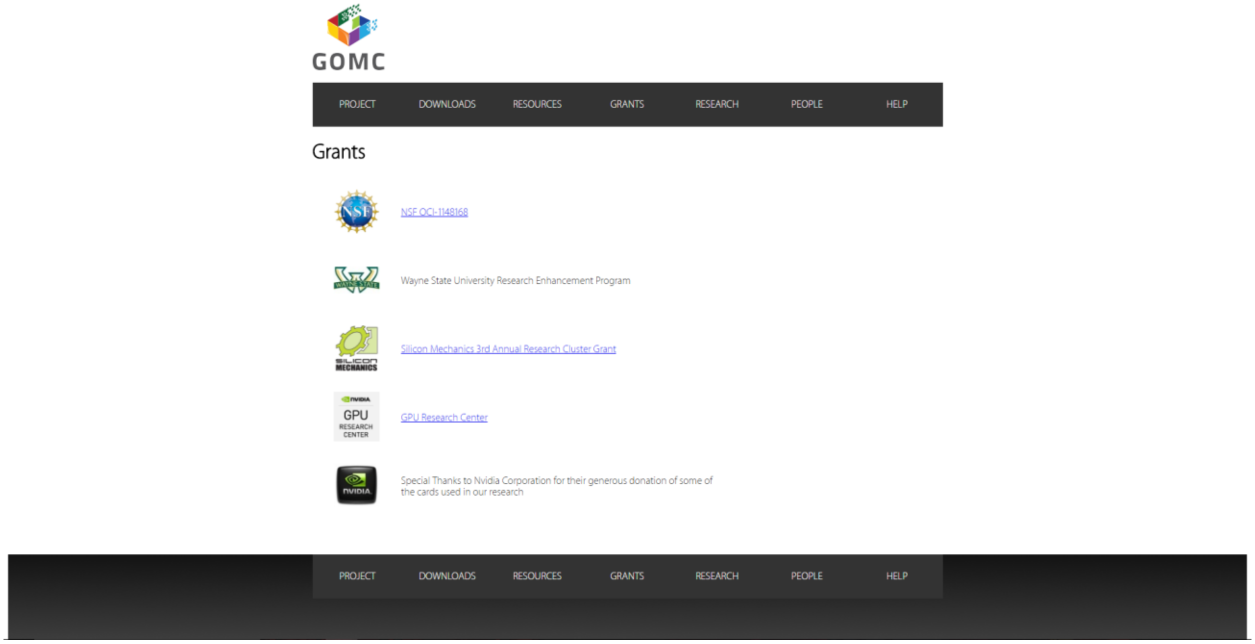
Eyad Hailat
Computer Science

Brock Jackman
Computer Science

Jason Mick
Chemical Engineering

Kamel Rushaidat
Computer Science

Grants



Grants

NSF OCI-1148168

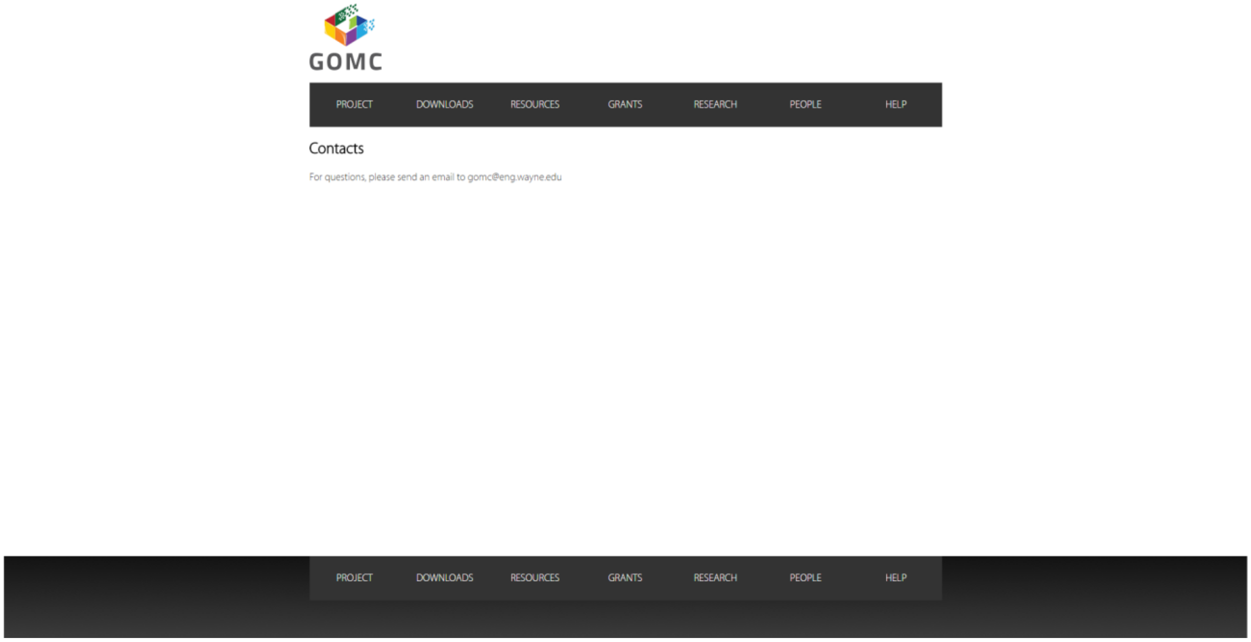
Wayne State University Research Enhancement Program

Silicon Mechanics 3rd Annual Research Cluster Grant

GPU Research Center

Special Thanks to Nvidia Corporation for their generous donation of some of the cards used in our research

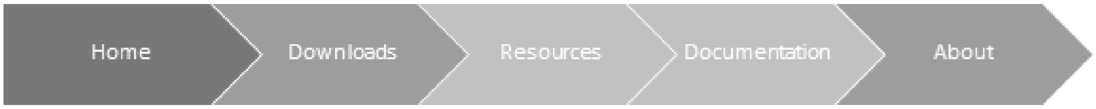
Contacts



Contacts

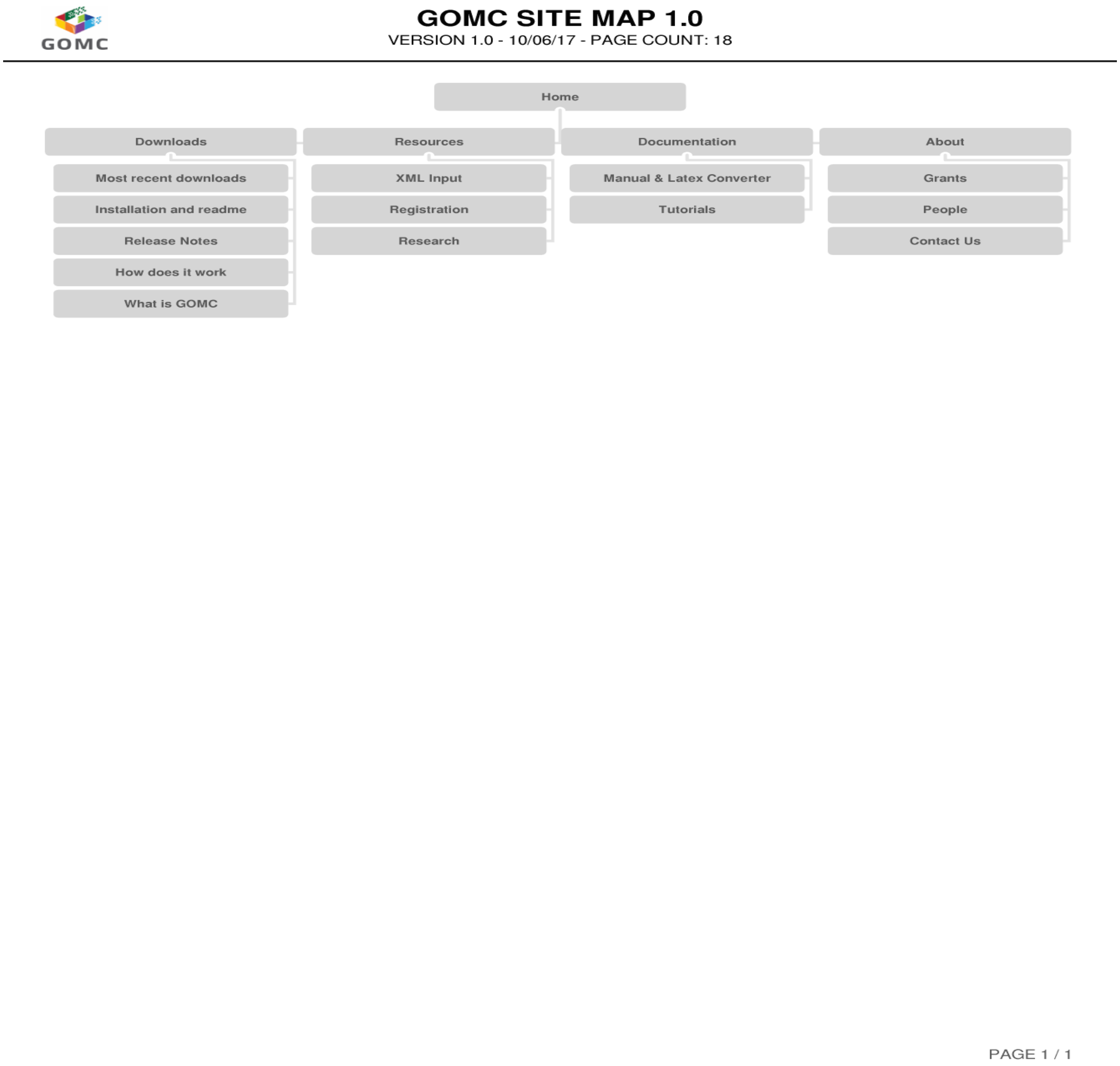
For questions, please send an email to gomc@eng.wayne.edu

In our implementation, we will use a streamlined menu to adopt a less complex navigation, search engine optimization and accessibility. Our full menu is not set in stone at the time of this revision as the client had multiple ideas for optimization currently it is set to be the following but this is subject to change.



The menu is structured in the conventional web standard of left to right with the leftmost item being the landing page upon navigating to the URL in a browser.

Like the navigation menu, the content of the website currently is not finalized the current site map may be modified in the very near future you can find it on the following page. The menu flows in the form of the home page being the landing page and having the main navigation. Each subsequent parent page will have its own navigation to inner content and parent navigation. As of this revision, the site map is still being actively worked on and the separation of child content into pages or as part of that page has not been laid out yet. It will be added in version 2.0 and version 3.0 is our anticipated final map which will include all links and endpoints according to our client's request.



The UI will conform to all standards and conventions produced by the tooling used to build the application which will be outlined in our Software Section. The UI will feature a responsive and clean design tailored for desktop and mobile support. It will follow accessibility standards and have the most optimal search engine optimization strategy that will be designed and implemented by the dev-team and approved by the client.

The first prototype will be built out in two versions: prototype-1-1 & prototype-1-2 correlating to p1 and p2 respectively. P1 will consist of a fully functioning site based off the scheme and layout provided by design 2. A screenshot is provided below and added to our appendix.

3.1.2 Hardware

In terms of system hardware this section has two main parts. The website and the simulation engine. The website does not have any required hardware to support its functionality. Once it is implemented it must render in modern desktops, laptops and mobile phones.
The simulation engine itself does have hardware limitations but those are fully outlined in the supporting documentation for the engine itself and will not be elaborated on in this section. Please view the formal documentation of the GOMC project:
http://gomc.eng.wayne.edu/GOMC_files/GOMC_Manual.pdf [4]

3.1.3 Software

The website will be built on ASP supporting the .Net architecture from Microsoft. The distribution version will contain razor html generated by html imports for each page. Bootstrap will the overall framework for the UI with custom component integration from materialize CSS. Both packages will be using vanilla JS and jQuery for dynamic page behavior and razor to support bound data from the server being loaded into the html.

Bootstrap will be the core framework for styling and accessibility, with a few components integrated from materialize CSS as needed. Materialize will only be used to supplement bootstrap capability and aim to allow for fully modernized components and is secondary to bootstrap.

Less CSS will be used to increase styling flexibility and create light-weight modules to prevent code bloat, add to readability and support optimal performance. JavaScript will be involved in the front-end with jQuery, AJAX, gulp.js and underscore.js. Each library serves a specific purpose to support the user experience on the front end. jQuery for DOM manipulation, AJAX for dynamically updating the downloads page and sending and receiving form data. Underscore for added functionality as needed and Gulp to automate distribution builds, by linting, validating, concatenating JS, and minifying CSS to result in the most optimal light-weight package.

For the backend, we are using Asp.Net/C# to handle communication with a SQL database as well as github (via the github API). For unit testing on the backend we will be using MS-Test to validate optimal functionality and on the front end we will be using QUnit on top of phantom JS to validate jQuery functionality, page performance and to simulate user paths. Currently our test suite is still up for discussion as the technology applied may be tweaked to provide the best experience.

3.1.4 Communication

Content delivery will follow standard HTTP protocol for client-server communication. Other than that, there is no present requirements around specific communication protocols now.

3.2 Functional Requirements

This section includes the functional requirements of the website.

3.2.0 Website

The purpose of the website is to provide a fully functional website for the GOMC team to present their work and show their work to the users. All requirements in this subsection are of the highest priority as the primary deliverable.

Table 3.2.0

ID	Related ID	Priority	Title	Description
3.2.0.1	null	1	Mockups	Six different mockups will be presented to client to narrow range of possible prototypes. **Acceptance Criteria** ● Client will see all mockups ● Client will pick which mockups they would like to see a prototype of ● Condense feedback of designs into supporting documents
3.2.0.2	3.2.0.1	1	Color Schema	Present different color schemes and get a final decision from the client **Acceptance Criteria** ● Multiple color palettes will be shown to the client which will provide a range of different combinations for website colors ● Client pick a 3-5 color combination and that will be the color scheme used in p11 & p22

3.2.0.3	3.2.0.1	1	Type Scheme	Present font-viewer.html with 24 combinations of web safe, modern readable font schemes and get a decision from the client **Acceptance Criteria** ● Font-test will present sample header and footer ● Font-test will present 2 fonts per 6 cards for an initial set of 12 combinations ● JavaScript will be applied to swap header and paragraph fonts doubling the total combinations to 24 ● Client will select at most 2 of the 24 combinations as the font-package for the website. This design choice will be rolled into P11 and P22
3.2.0.4	3.2.0.1-4	1	Prototype-1-1	Build and demonstrate P11. P11 must be based off the design of mockup 2, and include the functionality of all the related requirements. **Acceptance Criteria** ● Must have UV with client ● Must present all functionality in related requirements ● Feedback must be considered and documented
3.2.0.5	3.2.0.1-4	1	Prototype-1-2	Build and demonstrate p12. P12 must be based off the combination of the positive feedback from designs 3 and 6

				while aiming for a similar feel to design 4. The targeted functionality will be outlined in the Design Diagram in Appendix **Acceptance Criteria** ● Must have UV with client ● Must present all functionality in related requirements ● Feedback must be considered and documented
3.2.0.6	3.2.0.4-5	1	Menu design	Discuss different menu designs with client, implement feedback into both p11 and p22 **Acceptance Criteria** ● Must have UV with client ● Must present all functionality in related requirements ● Feedback must be considered and documented ● Feedback must be received and implemented in the final UV of p11 and p22

3.2.0.7	3.2.0.4-5	1	Content Hierarchy	Present site-map and discuss what will be on each page, how many pages there will be. And what can link to what page. **Acceptance Criteria** ● Must have UV with client ● Feedback must be considered and documented ● Feedback must be received and implemented in the final UV of p11 and p22
3.2.0.7	3.2.0.4-5	1	Footer design	Present 2 alternative footer designs to the client **Acceptance Criteria** ● Must have UV with to client ● Feedback must be considered and documented ● Feedback must be received and implemented in the final UV of p11 and p22
3.2.0.8	3.2.0.1-4	1	Final demo	Do a full UV with the client of both p11 and p12. Taking in new feedback to start P2 **Acceptance Criteria** ● Must have UV with client

				● Feedback must be considered and documented ● One design must be scrapped by the client’s choice ● The other will be expanded on for P2 deployed in the dev-server
3.2.0.10	3.2.0.7	1	Implement Support Pages	Tie in all main linked pages and start implementing content **Acceptance Criteria** ● Must have UV with client ● Feedback must be considered and documented ● Page content must be improved any bugs logged, assigned and tracked before P2 is presented
3.2.0.9	3.2.0.7	1	Prototype 2	P2 will have one version and it will run live in our dev environment as more features are added to it. **Acceptance Criteria** ● Must have UV with client ● Feedback must be considered and documented ● Any issues must be tracked as bugs as more features are rolled out

3.2.0.11	3.2.0.7	1	Implement core requirements	Implement main requirements established in further sections of this subsection **Acceptance Criteria** ● Must implement the new requirements outlined in document ● Bugs must be tracked and resolved ● UVs must occur weekly ● Dev-environment must be updated weekly

3.2.1 Downloads Page

The purpose of the downloads page is to provide a streamlined way for the user to download the latest released files of the GOMC program.

Table 3.2.1

ID	Related ID	Priority	Title	Description
3.2.1.1	null	1	Downloads Page	Allows the user to view and download the latest version of the GOMC program that is released in the github repo
3.2.1.2	3.2.1.1	2	Github API Releases	Creates a http GET request for the releases of the GOMC repo
3.2.1.3	3.2.1.2	2	Accept Github Response	Accepts the JSON response that GitHub returns with following 3.2.1.2
3.2.1.4	3.2.1.3	3	Parse JSON	Newtonsoft.Json will parse the JSON string input and convert to object

3.2.1.5	3.2.1.4	2	Create Downloads Model	Construct Downloads model with information about the release version and all file assets
3.2.1.6	3.2.1.1	1	Display Downloads	Show user latest release files as given by the Downloads Model

3.2.2 Config Forms Page

The config forms page will allow the user to specify input parameters for the config settings and after validation completes successfully, the user would then be able to download the result as an xml file to use with the GOMC program.

Table 3.2.2

ID	Related ID	Priority	Title	Description
3.2.2.1	null	1	Input Generator	Allow user to input config parameters and use with GOMC app.
3.2.2.2	3.2.2.1	1	Download Config XML	The user should be able to download the config input into an XML file.
3.2.2.3	3.2.2.2	1	Validation	All fields must be validated before the user can download the config file.
3.2.2.4	3.2.2.3	2	Integer Validation	Integer fields can only accept character input that range from ‘0’ to ‘9’.
3.2.2.5	3.2.2.3	2	Float Validation	Float fields can only accept character input that range from ‘0’ to ‘9’ and optionally a single ‘.’ character to signify the decimal point placement of the float value.
3.2.2.6	3.2.2.1	2	Enum Fields	Any field which is a string and can only be a specific value from a

				known list of values will be implemented as an enum.
3.2.2.7	3.2.2.6	2	Enum Radio	An enum field will be displayed to the user as a list of radio buttons where each radio button will represent a value of that enum.
3.2.2.8	3.2.2.6	4	Radio Label	Each radio input will have a text label naming it.
3.2.2.9	3.2.2.3	2	Number Value	All integer and float fields which have a maximum and/or minimum will be enforced as such on the user.
3.2.2.10	3.2.2.1	3	Field Label	Each field will be labeled with a name in the UI.
3.2.2.11	3.2.2.10	3	Field Popup	Upon hovering over a field, the user will be shown a UI popup which will describe that field.
3.2.2.12	3.2.2.2	2	Download XML button	Upon completing all fields and passing all validation, the user should be shown a download button which when clicked will download the XML config file.

3.3.3 Login System

The website will have a login system. The login system will allow a user to register and securely login. Users must pass the authentication process to successfully login. To complete and pass the authentication process, the supplied email and password must match a user’s email and password respectively.

Table 3.2.3

ID	Related ID	Priority	Title	Description
3.2.3.1	null	1	Login Authentication	The website will require authentication for a user to successfully login.
3.2.3.2	3.2.3.1	2	Registration	Users will be allowed to register to the website to login.
3.2.3.3	3.2.3.2	2	Register with Email	An email address is required to complete registration.
3.2.3.4	3.2.3.2	2	Register with Password	A password is required to complete registration.
3.2.3.5	3.2.3.2	1	Email Register Valid	The email supplied during registration must not match an email of other registered users.
3.2.3.6	3.2.3.1	3	Email Login	To authenticate a user during login, an email must be supplied.
3.2.3.7	3.2.3.1	3	Password Login	To authenticate a user during login, a password must be supplied.
3.2.3.8	3.2.3.1	1	Valid Email Authentication	For the authentication process to succeed, the supplied email must match an existing user's email.
3.2.3.9	3.2.3.8	1	Valid Password Authentication	For the authentication process to succeed, the supplied password must match the password of the user who is matched based on requirement 3.2.3.8.

3.3.4 Admin Page

The website will have an admin page. This page will require the user to login with an admin account. Admins can see valuable information in this page like the number of downloads or the regions in which users are using the program. Other information like the type of ensembles used by users will be shown.

Table 3.2.4

ID	Related ID	Priority	Title	Description
3.2.4.1	null	1	Admin View	There will be a page for admin related functionality.
3.2.4.2	3.2.4.1	1	Authentication	Only authenticated users can access the admin page.
3.2.4.3	3.2.4.2	1	Authorization	Authenticated users must have admin authorization to access the admin page.
3.2.4.4	3.2.4.2	3	Sign-In Request	A user who is unauthenticated will be requested to login.
3.2.4.5	3.2.4.3	3	Invalid Authorization	An authenticated user without admin authorization will be instructed to obtain admin privileges before being able to access the admin page.
3.2.4.6	3.2.4.1	1	Number of Downloads	Authenticated admins will be shown the number of downloads to the GOMC application.
3.2.4.7	3.2.4.1	2	Number of CPU based Apps	Authenticated admins will be shown the number of times the CPU based GOMC application has been executed by users.
3.2.4.8	3.2.4.7	2	Number of GPU based Apps	Authenticated admins will be shown the number of times the GPU based GOMC application has been executed by users.
3.2.4.9	3.2.4.1	2	Number of Windows based Apps	Authenticated admins will be shown the number of times the Windows version of the GOMC application has been executed by users.
3.2.4.10	3.2.4.1	2	Number of Linux based Apps	Authenticated admins will be shown the number of times the Linux version of the GOMC application has been executed by users.
3.2.4.11	3.2.4.1	2	Number of Mac based Apps	Authenticated admins will be shown the number of times the Mac version of the GOMC application

				has been executed by users.
3.2.4.12	3.2.4.1	2	Number of NVT based Apps	Authenticated admins will be shown the number of times the NVT version of the GOMC application has been executed by users.
3.2.4.13	3.2.4.1	2	Number of NPT based Apps	Authenticated admins will be shown the number of times the NPT version of the GOMC application has been executed by users.
3.2.4.14	3.2.4.1	2	Number of NVT Gibbs based Apps	Authenticated admins will be shown the number of times the NVT Gibbs version of the GOMC application has been executed by users.
3.2.4.15	3.2.4.1	2	Number of NPT Gibbs based Apps	Authenticated admins will be shown the number of times the NPT Gibbs version of the GOMC application has been executed by users.
3.3.4.16	3.2.6.1	2	LaTeX Upload	Allows an authenticated admin to upload a LaTeX file for the documentation which will then update the documentation of the website.

3.3.5 Config XML Parse

Table 3.2.5

ID	Related ID	Priority	Title	Description
3.2.5.1	null	1	Parse	The GOMC C++ application will have the ability to parse the XML

				input file and act upon those settings for processing.
3.2.5.2	3.2.5.1	2	Validation	To process the input file, the GOMC application must validate the input.
3.2.5.3	3.2.5.2	2	Valid XML	Only valid XML will be processed.
3.2.5.4	3.2.5.2	2	XML Schema Validation	An XML schema validation will occur before accepting the input file for processing.
3.2.5.5	3.2.5.3	3	Parse Fail Handling	When the user inputs a file which is not in XML format, they shall be informed their input file is not a valid XML file.
3.2.5.6	3.2.5.4	3	Invalid Schema Handling	Should the input file fail to succeed the XML schema validation, the user will be informed their input XML does not adhere to the required XML schema for the input file.
3.2.5.7	3.2.5.1	3	Error Output	In case of an error, the user will be informed in the console output.

3.3.6 LaTeX Converter

The website will have a functionality that is only available to admins which will allow for the conversion of a LaTeX document into HTML and PDF. The HTML output will be incorporated into the site itself and the PDF will be available for download.

Table 3.2.6

ID	Related ID	Priority	Title	Description
3.2.6.1	null	1	Conversion	The system will allow an admin to convert an existing LaTex document into HTML and PDF.
3.2.6.2	3.2.6.1	2	HTML sections	The output HTML must have each

				section as a separate page.
3.2.6.3	3.2.6.2	3	HTML Links	The output HTML will allow linking between sections.
3.2.6.4	3.2.6.1	2	Search	The output HTML will include a search functionality such that the user will be able to search keywords and shown results.
3.2.6.5	3.2.6.4	3	Search List Results	The results of a search will be displayed as a list to the user.
3.2.6.6	3.2.6.5	2	Search Results Item	Each list item in the search result will display the section name with appropriate link to said section and a short excerpt from that section which includes keyword(s) that are requested in the search.
3.2.6.7	3.2.6.3	2	PDF Links	The PDF output will include linking between different sections like that of the HTML output.
3.2.6.8	3.2.6.1	3	PDF Download	The PDF output will be available for download to the user.

3.3 Non-Functional Requirements

This section will detail all requirements which are not functional.

3.3.1 Performance

It is required to have the website adhere to our performance requirements. Failing to do some can lead to issues with downtime and reliability in general. The overall requirements related to performance include things like ram usage, disk usage, page load time, and concurrent users.

Table 3.3.1

ID	Related ID	Priority	Title	Description

3.3.1.1	null	2	Page Load Time	A request to load a page will not exceed 5 seconds before the page fully loads.
3.3.1.2	null	1	Web Site Storage	The hard drive storage space required to run the website will remain below 30 GB.
3.3.1.3	null	1	Web Site Ram	The memory space required to run the website will not exceed 1GB
3.3.1.4	null	2	User Count	The website must support 100 concurrent users.

3.3.2 Reliability

The website should be reliable. This means that if there are a few hours of downtime. In addition, it would be beneficial for the overall reliability to have the number of bugs reported, or discovered through debugging, to be low compared to the lines of code of the website.

Table 3.3.2

ID	Related ID	Priority	Title	Description
3.3.2.1	3.3.3.1	2	Downtime	The website will not have a downtime greater than 1 hour.
3.3.2.2	null	3	Bug Count	The software for the website will have fewer than 5 bugs per 1000 lines of code.

3.3.3 Availability

Overall, the website should be operational. However, there needs to be a scheduled maintenance time which should remain consistent so the user can expect it rather than come as a surprise.

At the time of maintenance, the website needs to be unavailable so that maintenance related tasks, which would require the site to be unavailable, can be completed. An example of such tasks would be to change database schemas or table structure. This cannot be done if the site is running and thus the site must be offline at that time.

Table 3.3.3

ID	Related ID	Priority	Title	Description
3.3.3.1	null	1	Availability	The website will be available and running correctly 90% of the time.
3.3.3.2	3.3.3.2	4	Maintenance	Two hours for one day of the week will be dedicated for maintenance work and in that period the web site will not be available.

3.3.4 Security

The website's security requirements will be dictated by a security standard which is complaint to what is well-known security practices. This security standard is defined by following table.

Table 3.3.4

ID	Related ID	Priority	Title	Description
3.3.4.1	null	1	Enforce Security Standards	The website must adhere to well-known and understood security standards
3.3.4.2	3.3.4.1	1	Authentication for Admin Page	The website must have a login system to authenticate a user for accessing the admin page.
3.3.4.3	3.3.4.2	2	Authorization for Admin Page	Only authenticated and authorized admins can access the admin page and use its functionality.
3.3.4.4	3.3.4.1	1	Passwords Hashed	All passwords saved in the database

				must be hashed with the SHA-2 256 algorithm.

3.3.5 Maintainability

As indicated in 3.3.3, the website will also include maintenance. During times of maintenance, webmasters and developers can clean up and change the database as needed. Maintenance work include changes to table layout or other changes to the database due to a release of a new feature.

3.3.6 Portability

The website and database must be portable. This means that at any time, the database or website can be switched to a different host without losing functionality or data.

3.4 Design Constraints

The development website is hosted in EC2 with Amazon Web Services (AWS). The instance is a t2. micro and the OS is Windows 2012 Server. Only 1GB of ram is allocated to that instance. In addition, the hard drive space is limited to 30GB. The processor is of the Intel Xeon family with 1 vCPU clocked at 2.5 GHz.

The CPU processing required to run the website shall not exceed the limits set by the t2. micro instance. The total hard disk space required to run and maintain the web site should not be greater than 30 GB.

3.5 Logical Database Requirements

The development website has a dedicated database server. The server is hosted with Amazon Relational Database Service (RDS). The server chosen is Microsoft’s SQL Server Express Edition. A 20GB storage limit is imposed on the instance.

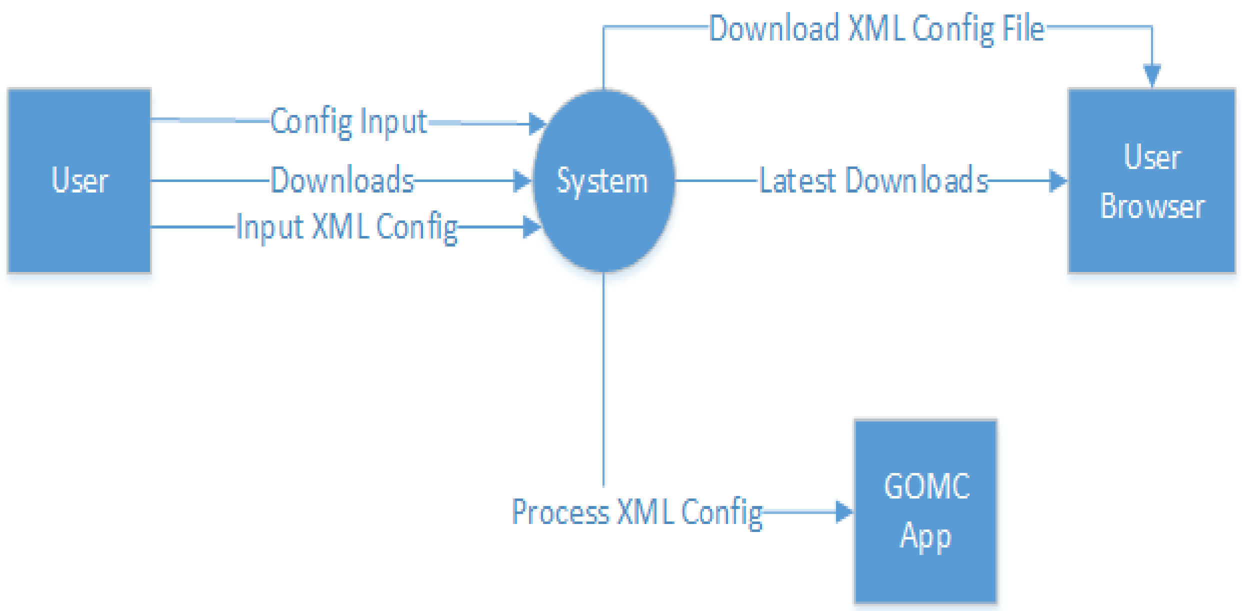
The total storage needs the database of the website shall not exceed 20GB.

4. Analysis Models

4.1 Data Flow Diagrams (DFD)

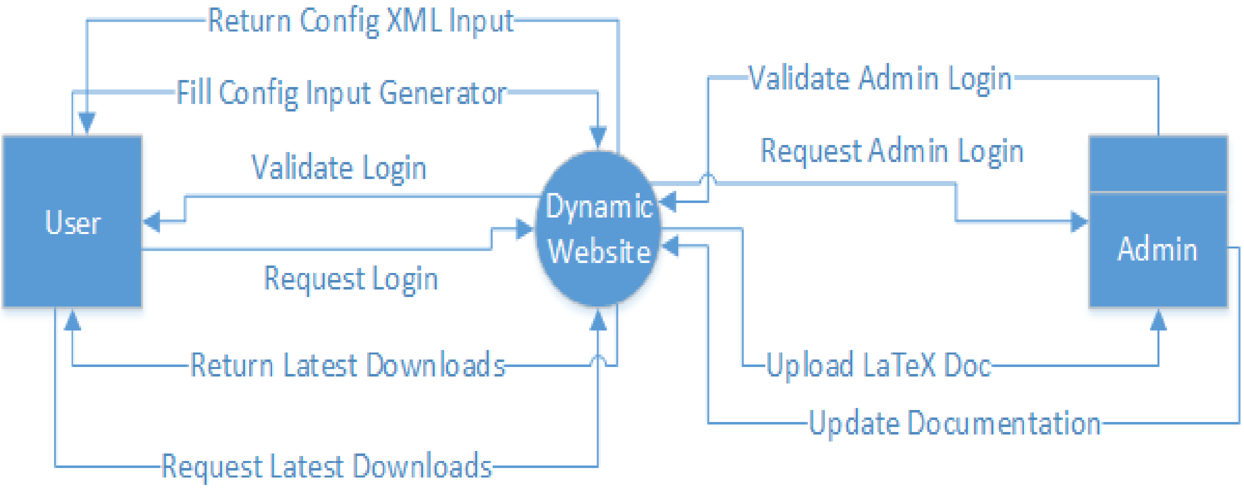
4.1.1 System DFD

Level 0 DFD for whole the System



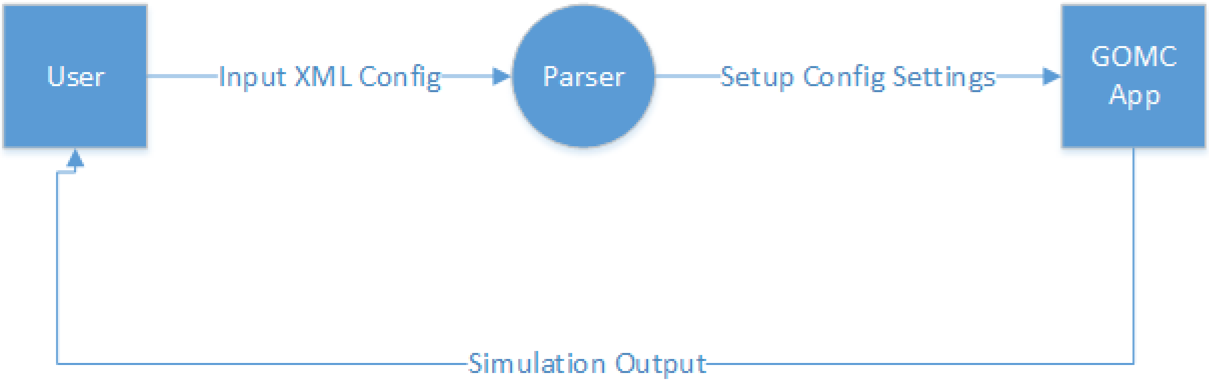
4.1.2 Website DFD

Level 1 DFD for Website



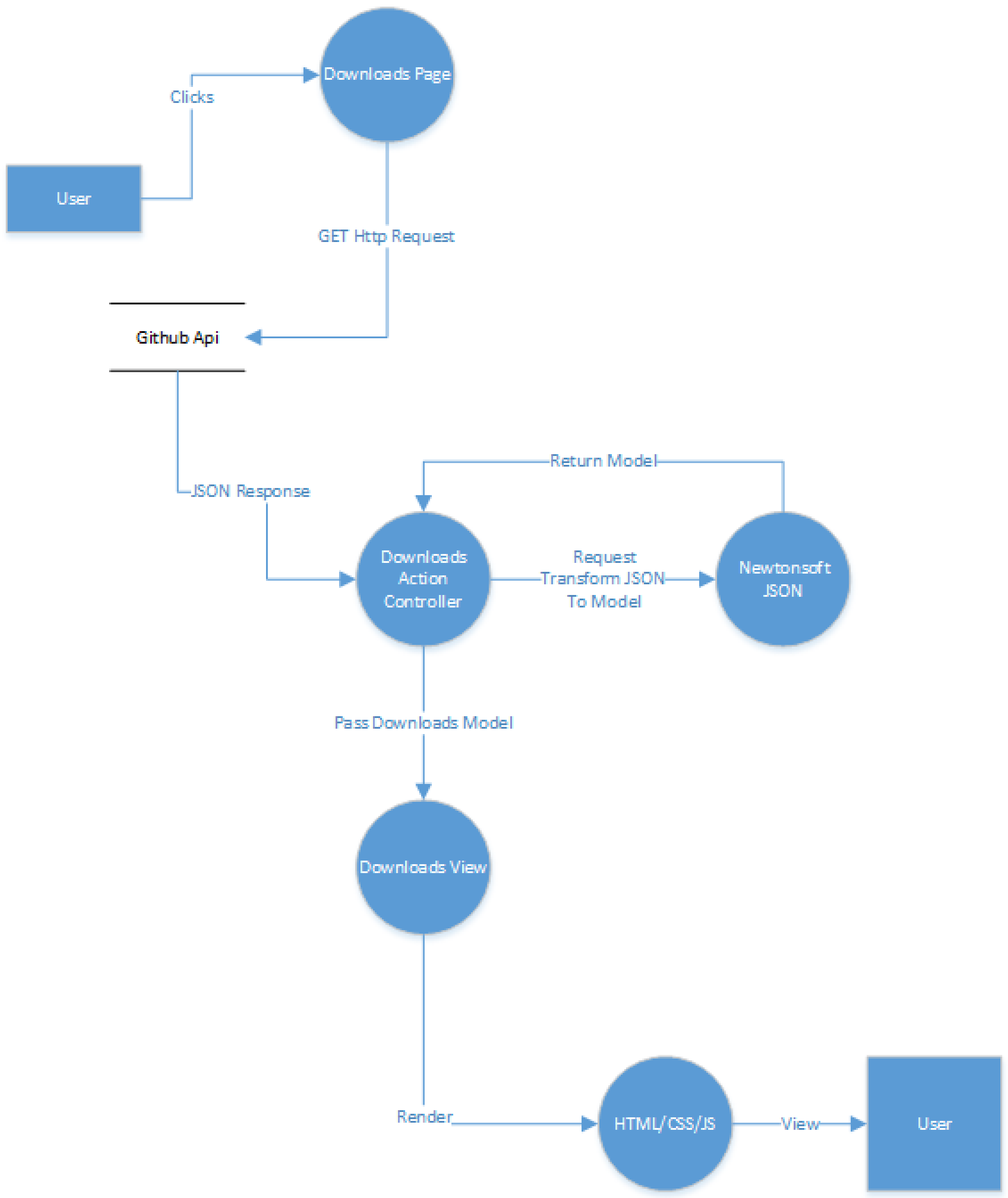
4.1.3 Parser DFD

Level 1 for XML Parser



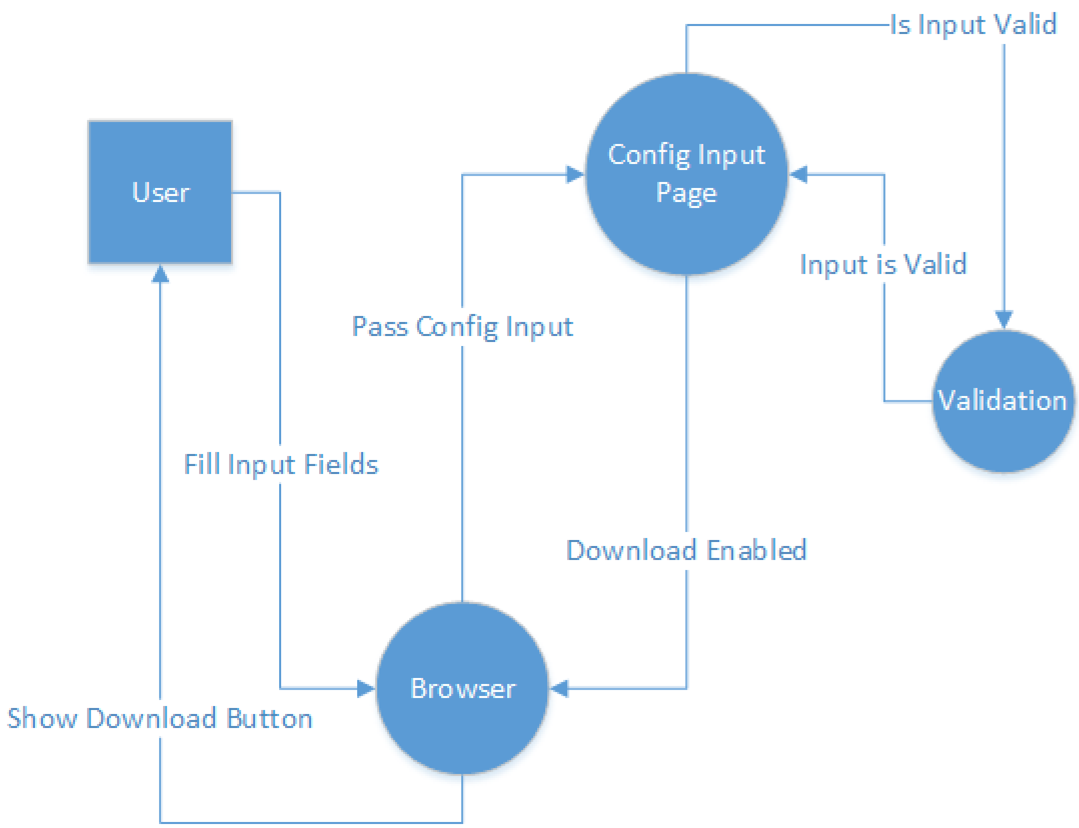
4.1.4 Downloads Page DFD

Level 2 DFD for Downloads Page

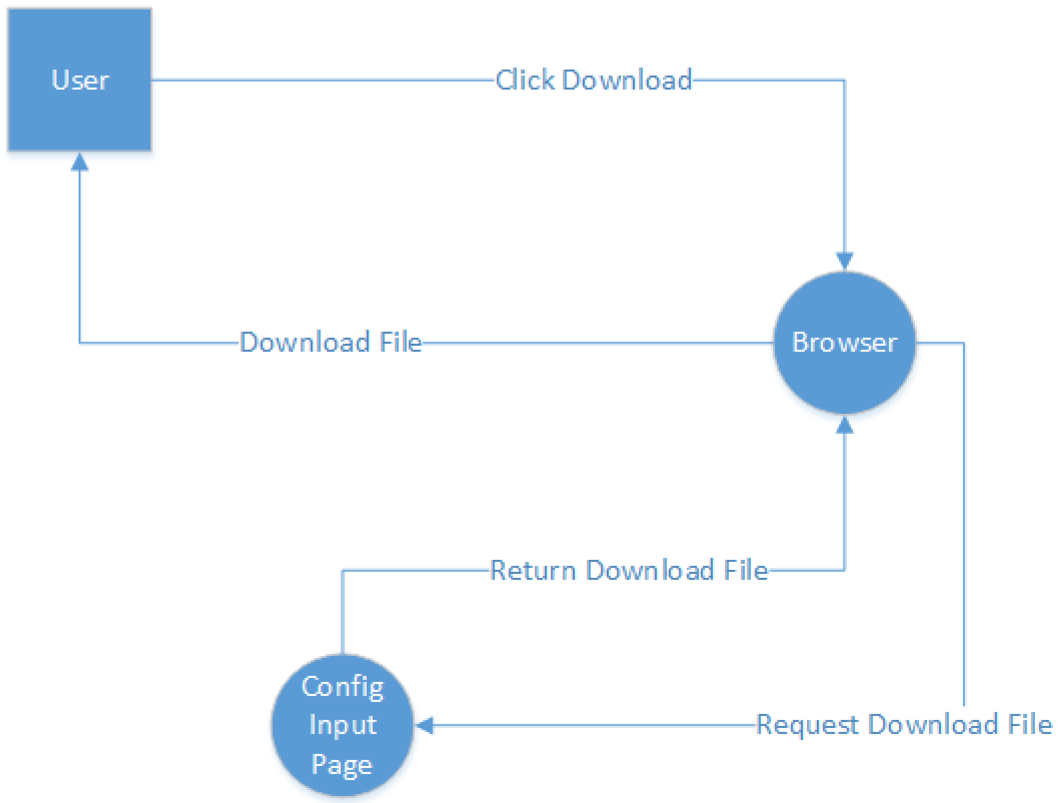


4.1.5 Config Page DFD

Level 2 DFD for Config Page



Level 1 DFD for Download Click


User
Click Download
Browser
Download File
Return Download File
Config Input Page
Request Download File

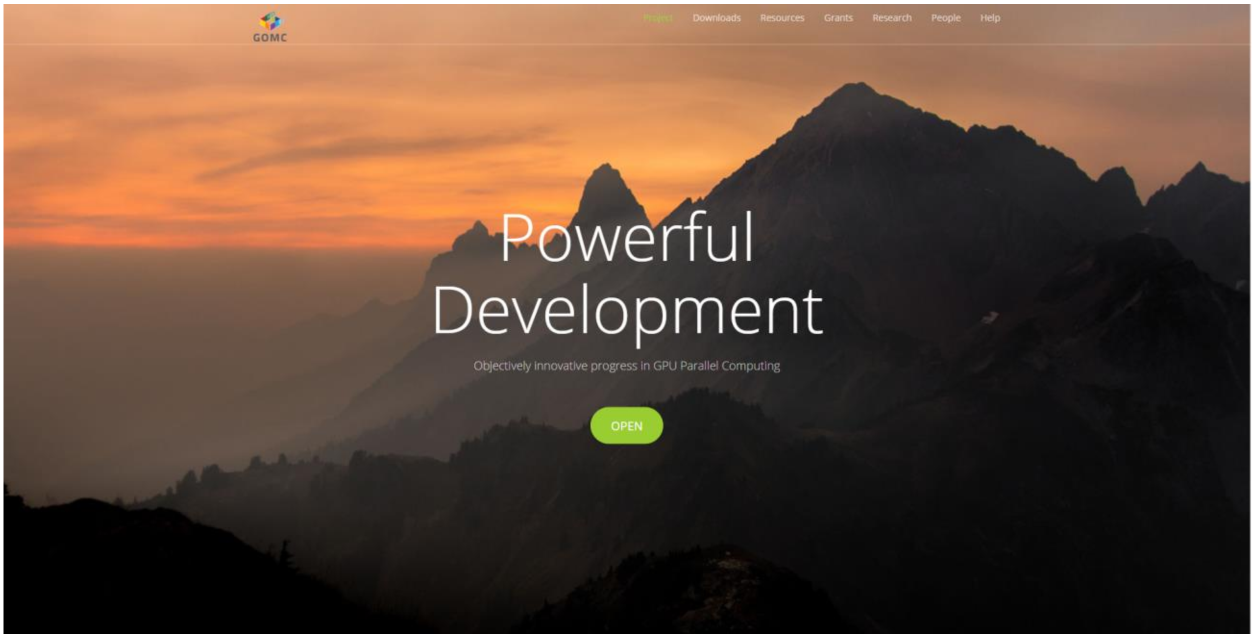
Appendix A

This section will entail a comprehensive set of supporting documents, files, mockups, designs and any supporting documents that the team has produced to supplement the understanding and development of this project.

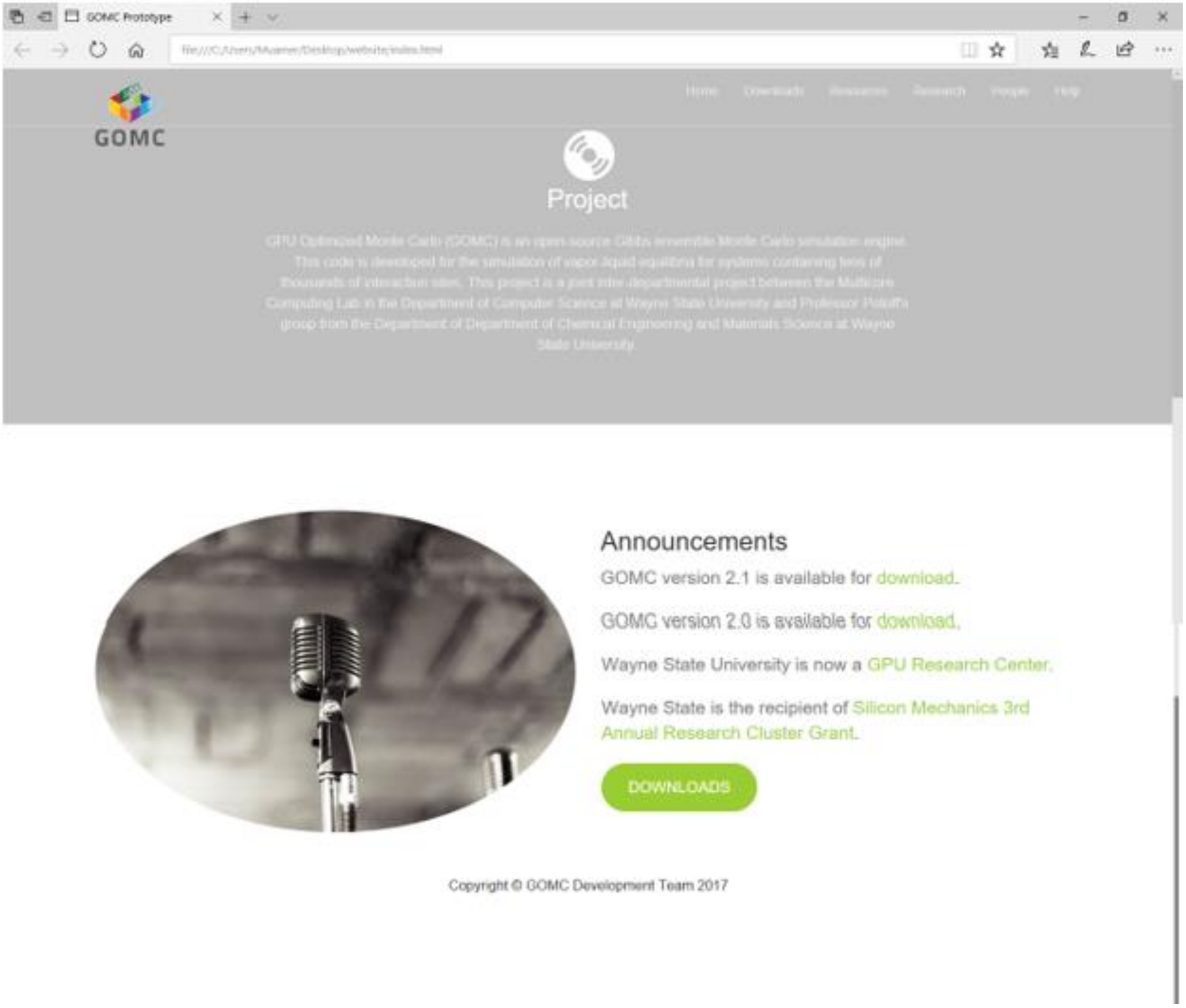
Website Prototype-1-1

Design of Prototype-1-1 was heavily inspired by the content of "Mock-up 2", the feedback from the client and implementation of a few changes such as getting rid of the background image and making the overall website seem simpler with a clean look. The custom style sheet from "Mock-up 2" was used with the rest of the pages that way the layout is flowing throughout each page. We incorporated the information from the current GOMC website into the prototype and from here we will continue to change the design/layout according to the client's likings.

Mock-up 2



Home page view



Project

GPU Optimized Monte Carlo (GOMC) is an open-source Gibbs ensemble Monte Carlo simulation engine. This code is developed for the simulation of vapor-liquid equilibria for systems containing tens of thousands of interaction sites. This project is a joint inter-departmental project between the Multicore Computing Lab in the Department of Computer Science at Wayne State University and Professor Potoff's group from the Department of Department of Chemical Engineering and Materials Science at Wayne State University.

Announcements

GOMC version 2.1 is available for download.

GOMC version 2.0 is available for download.

Wayne State University is now a GPU Research Center.

Wayne State is the recipient of Silicon Mechanics 3rd Annual Research Cluster Grant.

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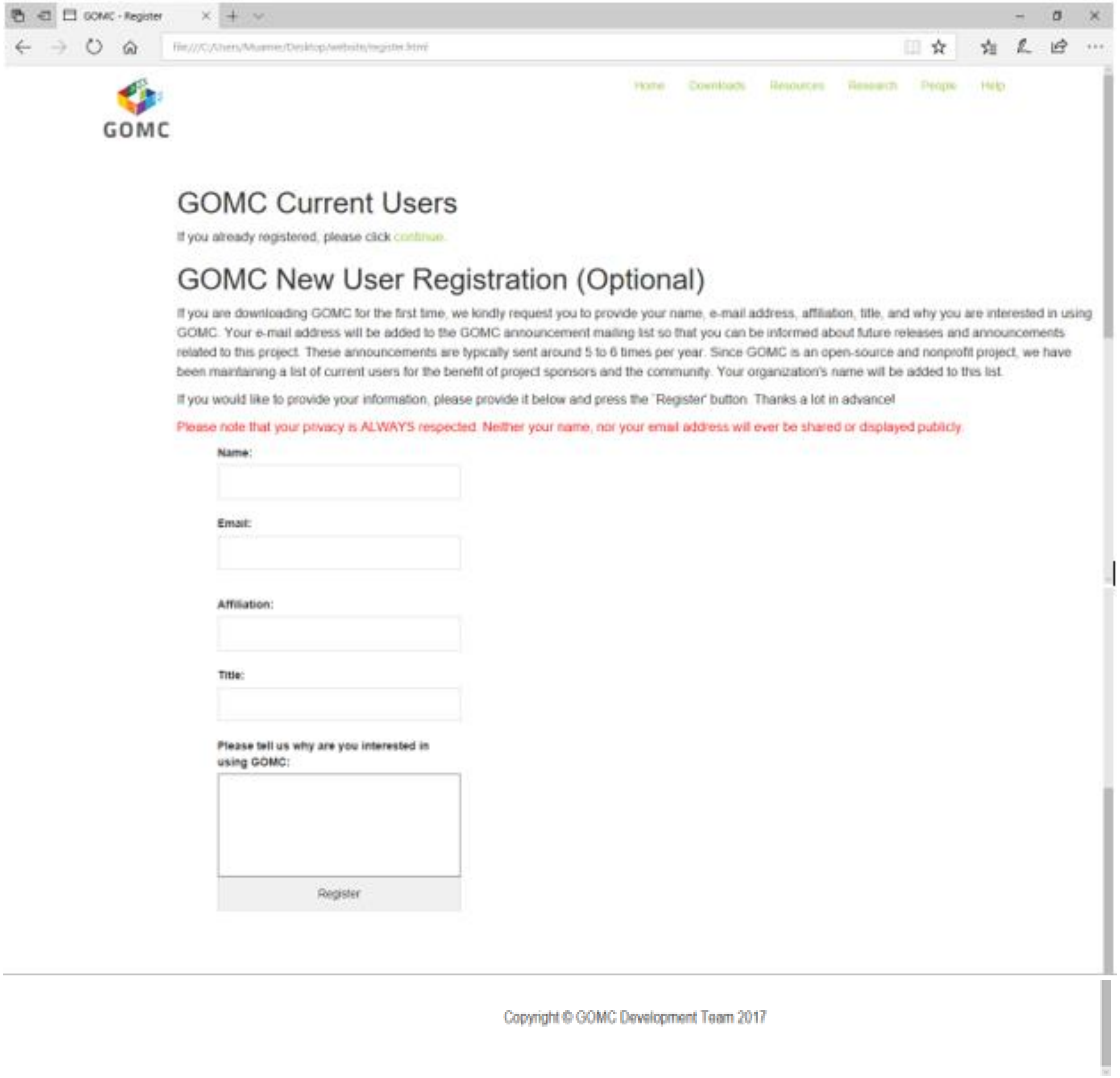
Downloads page view



GOMC Current Users

If you already registered, please click continue.

GOMC New User Registration (Optional)

If you are downloading GOMC for the first time, we kindly request you to provide your name, e-mail address, affiliation, title, and why you are interested in using GOMC. Your e-mail address will be added to the GOMC announcement mailing list so that you can be informed about future releases and announcements related to this project. These announcements are typically sent around 5 to 6 times per year. Since GOMC is an open-source and nonprofit project, we have been maintaining a list of current users for the benefit of project sponsors and the community. Your organization's name will be added to this list.

If you would like to provide your information, please provide it below and press the 'Register' button. Thanks a lot in advance!

Please note that your privacy is ALWAYS respected. Neither your name, nor your email address will ever be shared or displayed publicly.

Name:

Email:

Affiliation:

Title:

Please tell us why are you interested in using GOMC:

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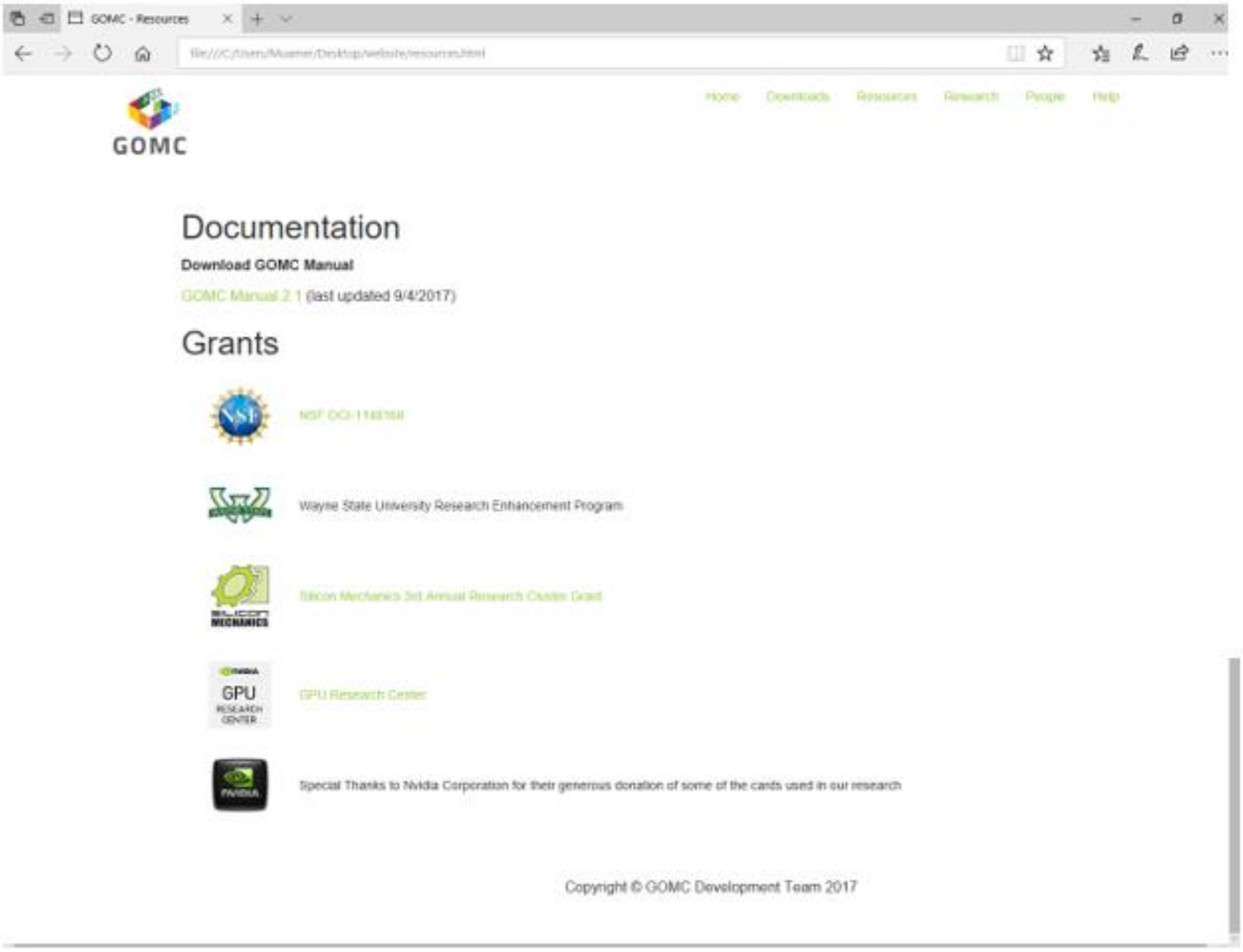
Resources page view



Documentation

Download GOMC Manual

GOMC Manual 2.1 (last updated 9/4/2017)

Grants

NSF OCI-1148168

Wayne State University Research Enhancement Program

Silicon Mechanics 3rd Annual Research Cluster Grant

GPU Research Center

Special Thanks to Nvidia Corporation for their generous donation of some of the cards used in our research

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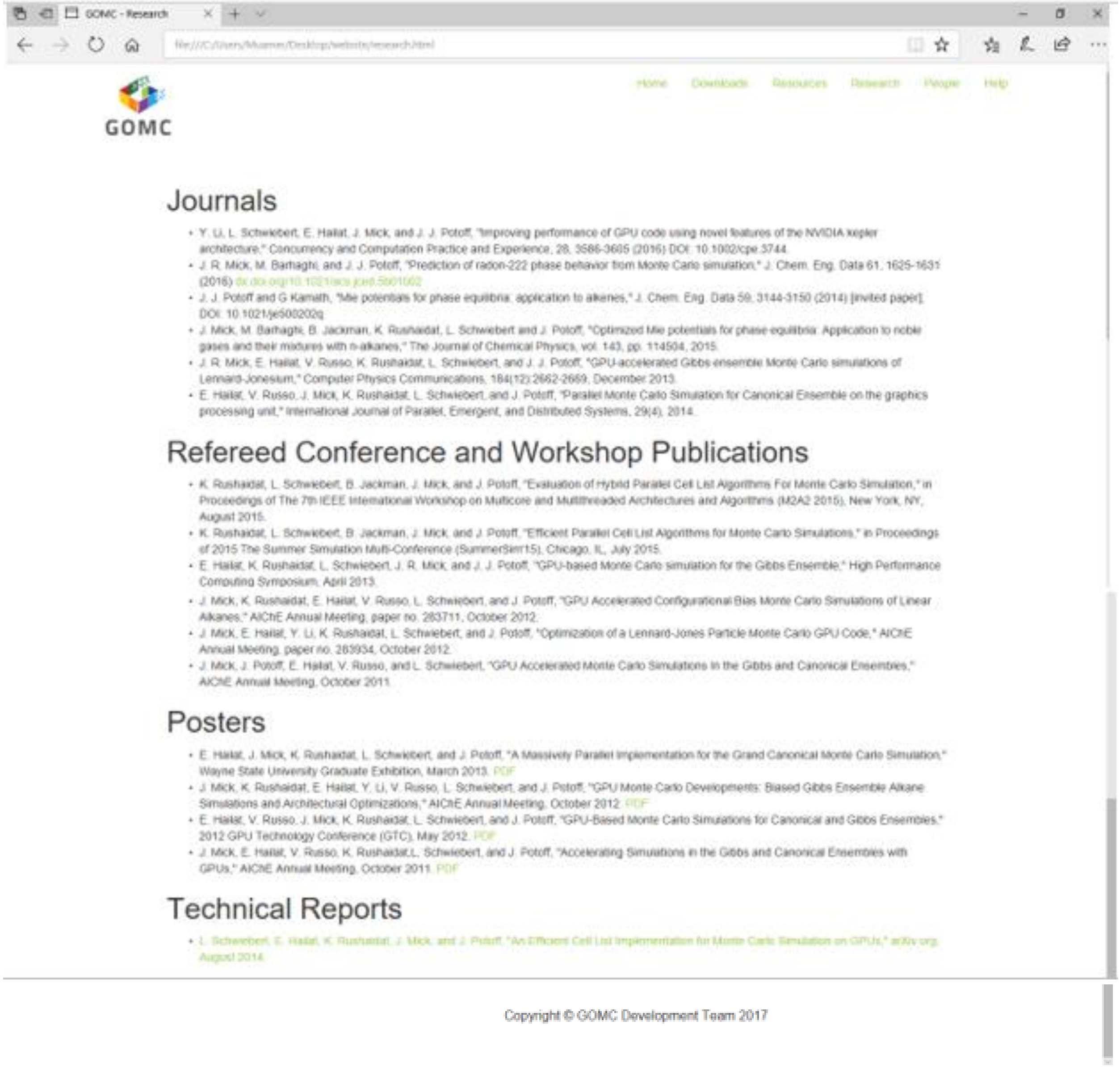
Research page view



Journals

- Y. Li, L. Schwiebert, E. Hailat, J. Mick, and J. J. Potoff, "Improving performance of GPU code using novel features of the NVIDIA kepler architecture," Concurrency and Computation Practice and Experience, 28, 3586-3605 (2016) DOI: 10.1002/cpe.3744
- J. R. Mick, M. Barhaghi, and J. J. Potoff, "Prediction of radon-222 phase behavior from Monte Carlo simulation," J. Chem. Eng. Data 61, 1625-1631 (2016) dx.doi.org/10.1021/acs.jced.5b01002
- J. J. Potoff and G Kamath, "Mie potentials for phase equilibria: application to alkenes," J. Chem. Eng. Data 59, 3144-3150 (2014) [invited paper]. DOI: 10.1021/je500202q
- J. Mick, M. Barhaghi, B. Jackman, K. Rushaidat, L. Schwiebert and J. Potoff, "Optimized Mie potentials for phase equilibria: Application to noble gases and their mixtures with n-alkanes," The Journal of Chemical Physics, vol. 143, pp. 114504, 2015.
- J. R. Mick, E. Hailat, V. Russo, K. Rushaidat, L. Schwiebert, and J. J. Potoff, "GPU-accelerated Gibbs ensemble Monte Carlo simulations of Lennard-Jonesium," Computer Physics Communications, 184(12):2662-2669, December 2013.
- E. Hailat, V. Russo, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "Parallel Monte Carlo Simulation for Canonical Ensemble on the graphics processing unit," International Journal of Parallel, Emergent, and Distributed Systems, 29(4), 2014.

Refereed Conference and Workshop Publications

- K. Rushaidat, L. Schwiebert, B. Jackman, J. Mick, and J. Potoff, "Evaluation of Hybrid Parallel Cell List Algorithms For Monte Carlo Simulation," in Proceedings of The 7th IEEE International Workshop on Multicore and Multithreaded Architectures and Algorithms (M2A2 2015), New York, NY, August 2015.
- K. Rushaidat, L. Schwiebert, B. Jackman, J. Mick, and J. Potoff, "Efficient Parallel Cell List Algorithms for Monte Carlo Simulations," in Proceedings of 2015 The Summer Simulation Multi-Conference (SummerSim'15), Chicago, IL, July 2015.
- E. Hailat, K. Rushaidat, L. Schwiebert, J. R. Mick, and J. J. Potoff, "GPU-based Monte Carlo simulation for the Gibbs Ensemble," High Performance Computing Symposium, April 2013.
- J. Mick, K. Rushaidat, E. Hailat, V. Russo, L. Schwiebert, and J. Potoff, "GPU Accelerated Configurational Bias Monte Carlo Simulations of Linear Alkanes," AIChE Annual Meeting, paper no. 283711, October 2012.
- J. Mick, E. Hailat, Y. Li, K. Rushaidat, L. Schwiebert, and J. Potoff, "Optimization of a Lennard-Jones Particle Monte Carlo GPU Code," AIChE Annual Meeting, paper no. 283934, October 2012.
- J. Mick, J. Potoff, E. Hailat, V. Russo, and L. Schwiebert, "GPU Accelerated Monte Carlo Simulations in the Gibbs and Canonical Ensembles," AIChE Annual Meeting, October 2011.

Posters

- E. Hailat, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "A Massively Parallel Implementation for the Grand Canonical Monte Carlo Simulation," Wayne State University Graduate Exhibition, March 2013. PDF
- J. Mick, K. Rushaidat, E. Hailat, Y. Li, V. Russo, L. Schwiebert, and J. Potoff, "GPU Monte Carlo Developments: Biased Gibbs Ensemble Alkane Simulations and Architectural Optimizations," AIChE Annual Meeting, October 2012. PDF
- E. Hailat, V. Russo, J. Mick, K. Rushaidat, L. Schwiebert, and J. Potoff, "GPU-Based Monte Carlo Simulations for Canonical and Gibbs Ensembles," 2012 GPU Technology Conference (GTC), May 2012. PDF
- J. Mick, E. Hailat, V. Russo, K. Rushaidat,L. Schwiebert, and J. Potoff, "Accelerating Simulations in the Gibbs and Canonical Ensembles with GPUs," AIChE Annual Meeting, October 2011. PDF

Technical Reports

- L. Schwiebert, E. Hailat, K. Rushaidat, J. Mick, and J. Potoff, "An Efficient Cell List Implementation for Monte Carlo Simulation on GPUs," arXiv.org, August 2014.

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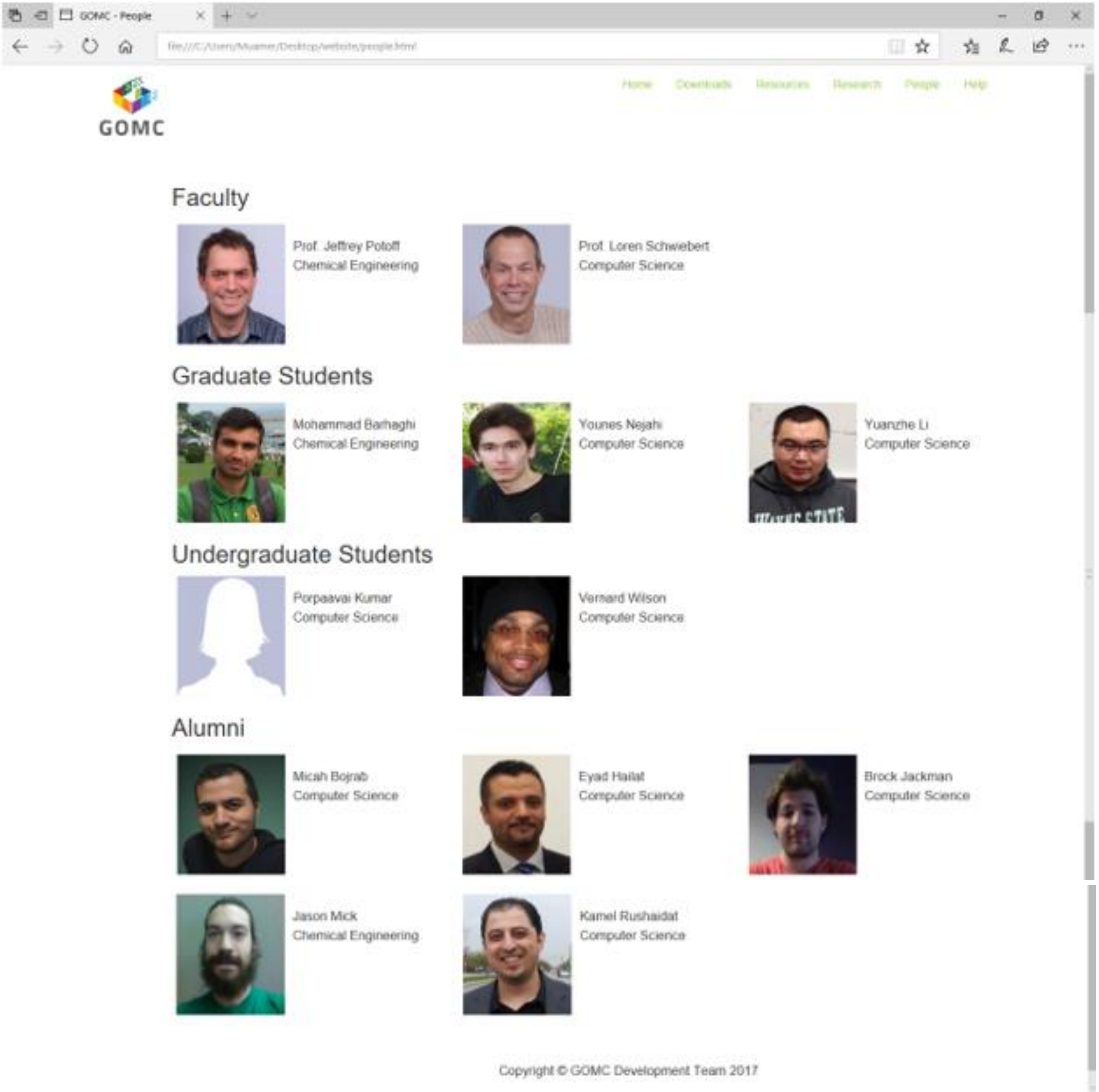
People page view



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Chemical Engineering

Younes Nejahi
Computer Science

Yuanzhe Li
Computer Science

Undergraduate Students

Porpaavai Kumar
Computer Science

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Computer Science

Alumni

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Computer Science

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Computer Science

Brock Jackman
Computer Science

Jason Mick
Chemical Engineering

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Computer Science

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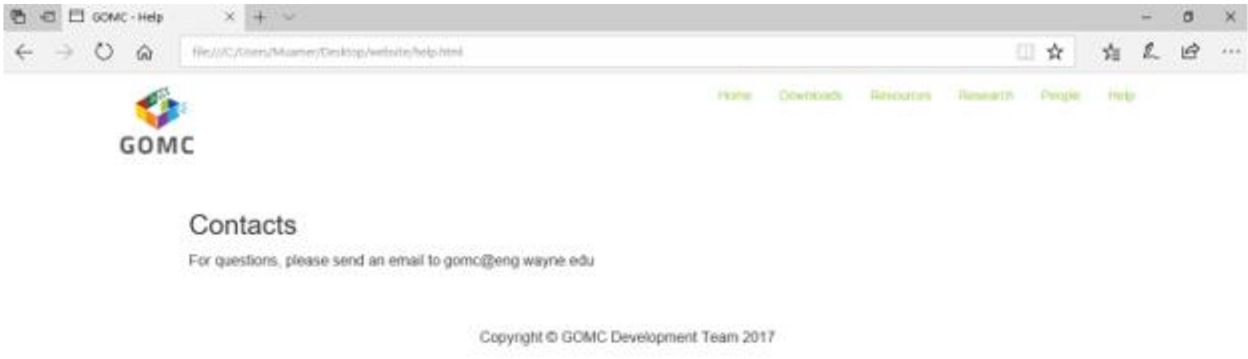
Help page view



Contacts

For questions, please send an email to gomc@eng wayne edu

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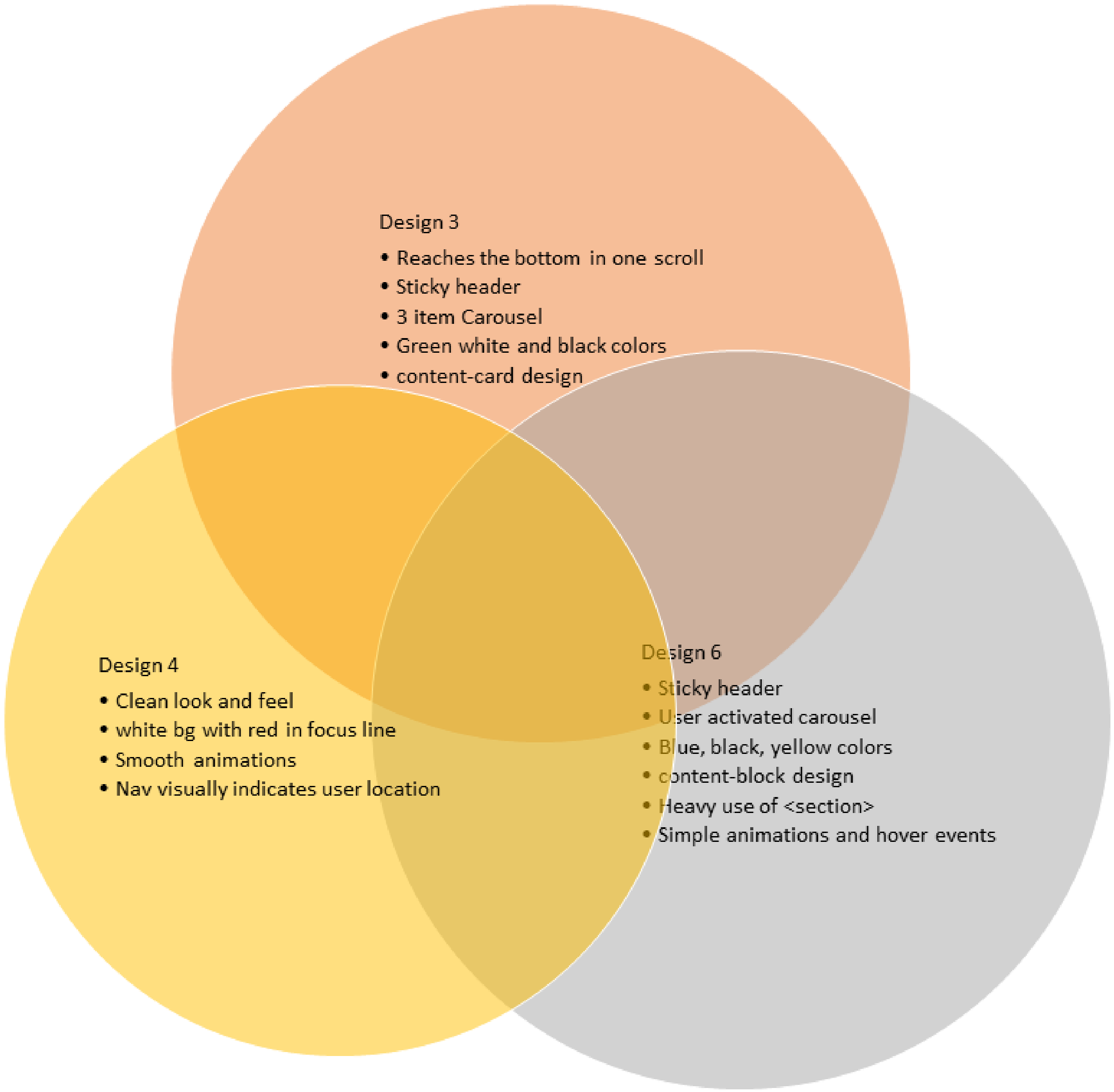
Design Diagram Prototype-1-2



Design 3

- Reaches the bottom in one scroll
- Sticky header
- 3 item Carousel
- Green white and black colors
- content-card design

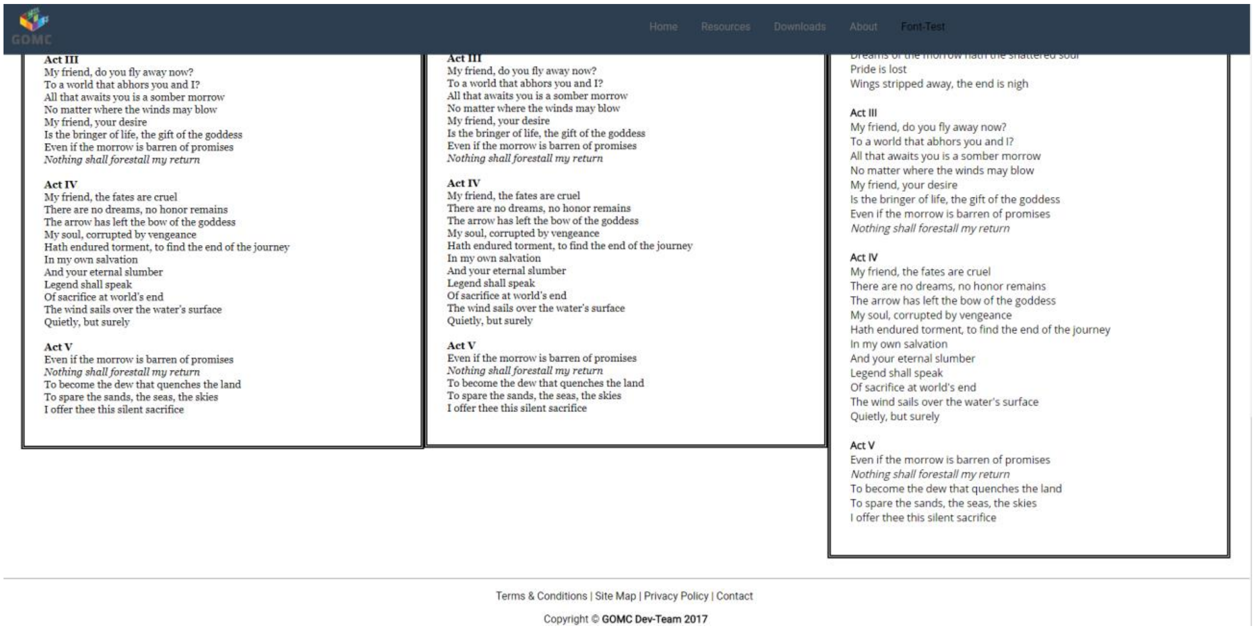
Design 4

- Clean look and feel
- white bg with red in focus line
- Smooth animations
- Nav visually indicates user location

Design 6

- Sticky header
- User activated carousel
- Blue, black, yellow colors
- content-block design
- Heavy use of <section>
- Simple animations and hover events

Font-Test Sticky header, new navbar and new footer Prototype-1-2



Act III
My friend, do you fly away now?
To a world that abhors you and I?
All that awaits you is a somber morrow
No matter where the winds may blow
My friend, your desire
Is the bringer of life, the gift of the goddess
Even if the morrow is barren of promises
Nothing shall forestall my return

Act IV
My friend, the fates are cruel
There are no dreams, no honor remains
The arrow has left the bow of the goddess
My soul, corrupted by vengeance
Hath endured torment, to find the end of the journey
In my own salvation
And your eternal slumber
Legend shall speak
Of sacrifice at world's end
The wind sails over the water's surface
Quietly, but surely

Act V
Even if the morrow is barren of promises
Nothing shall forestall my return
To become the dew that quenches the land
To spare the sands, the seas, the skies
I offer thee this silent sacrifice

Act III
My friend, do you fly away now?
To a world that abhors you and I?
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Pride is lost
Wings stripped away, the end is nigh

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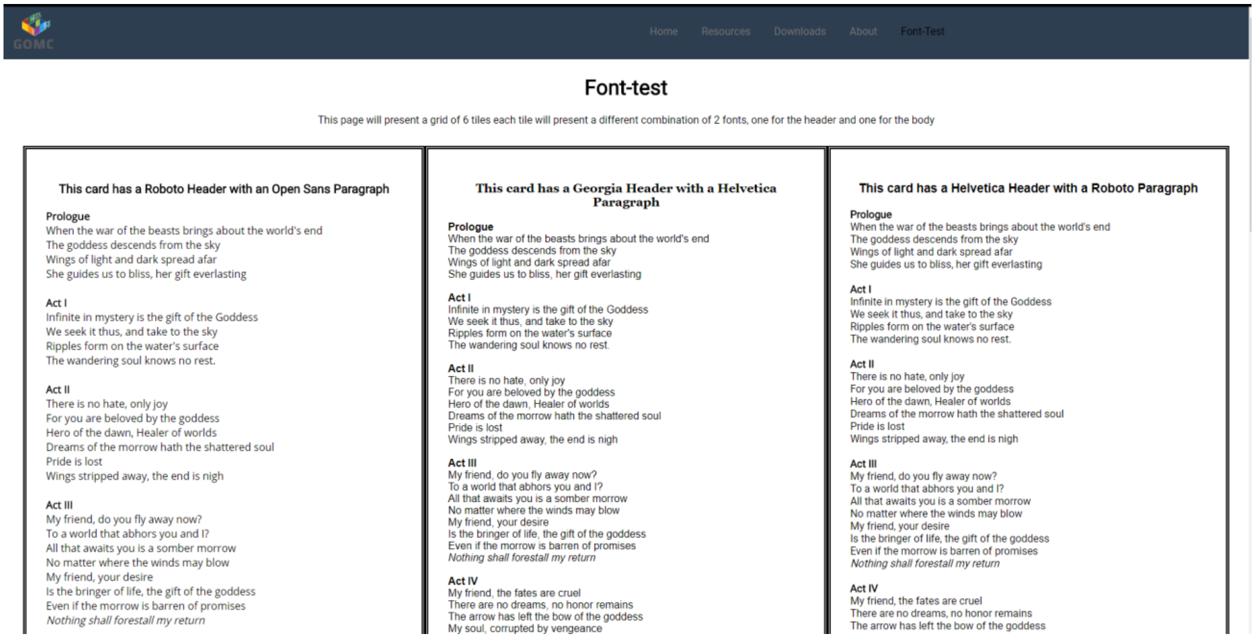
Font-Test.html- Prototype-1-2



Font-test

This page will present a grid of 6 tiles each tile will present a different combination of 2 fonts, one for the header and one for the body

This card has a Roboto Header with an Open Sans Paragraph

Prologue
When the war of the beasts brings about the world's end
The goddess descends from the sky
Wings of light and dark spread afar
She guides us to bliss, her gift everlasting

Act I
Infinite in mystery is the gift of the Goddess
We seek it thus, and take to the sky
Ripples form on the water's surface
The wandering soul knows no rest.

Act II
There is no hate, only joy
For you are beloved by the goddess
Hero of the dawn, Healer of worlds
Dreams of the morrow hath the shattered soul
Pride is lost
Wings stripped away, the end is nigh

Act III
My friend, do you fly away now?
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My friend, your desire
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Even if the morrow is barren of promises
Nothing shall forestall my return

This card has a Georgia Header with a Helvetica Paragraph

Prologue
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Even if the morrow is barren of promises
Nothing shall forestall my return

Act IV
My friend, the fates are cruel
There are no dreams, no honor remains
The arrow has left the bow of the goddess
My soul, corrupted by vengeance

This card has a Helvetica Header with a Roboto Paragraph

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Act IV
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There are no dreams, no honor remains
The arrow has left the bow of the goddess

User Profile Report v 1.0

Persona

Name: R
Age: 23-35
Typical Day: Lots of time reading papers, running experiments, supporting faculty
Skills: Varying based off computer science/chemical engineering background
Tools & Knowledge: GPU programming terms, molecular simulation terms
Reports To: Some University Faculty, doesn’t have anyone reporting to them

Temperament & Empathy

· Educated: Completed undergraduate degree in computer science or chemical engineering possibly even a master. Knows their area of expertise very well.

▪ Impatient: R is an up and coming leader in the technical age, following millennial conventions R has a world of info readily available so taking the time to use ours needs to be concise.

· Practical: This isn’t something to read about for fun. It’s something that the R needs to find, install, run and use in day to day work. Having concise material, and ease of navigation would be best for R.

Navigation Cases

Case 1: R wants Download
When the page loads they will a see an icon at the center of the page with the 3 most recent downloads

Case 2: R wants to learn about the project
On page load immediately left of the downloads will be a card that has text that entices them to click it. On click they will be redirected to a new page with a high-level overview, high-light strong points of the software, technical documentation, and examples

Case 3: User wants to talk to someone about joining or has questions
Navbar is always present on scroll and on the right-hand side there is a support button that the user can click. Which will give them content to meet their need

Navbar Designs

The navigation menu is another area of redesign. Each version of prototype 1 will implement a different design until we can receive a final confirmation from our client. The navigation bar is a big proponent of user experience and a very important part of our redesign.

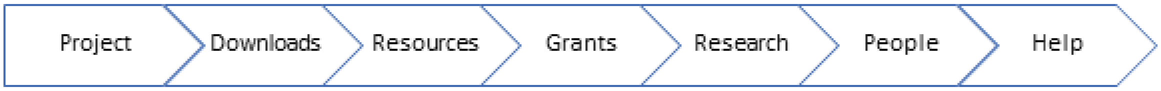
Menu Condensing Strategy

Our goal is to keep the navigation bar under 5 Menu items to condense are the following:

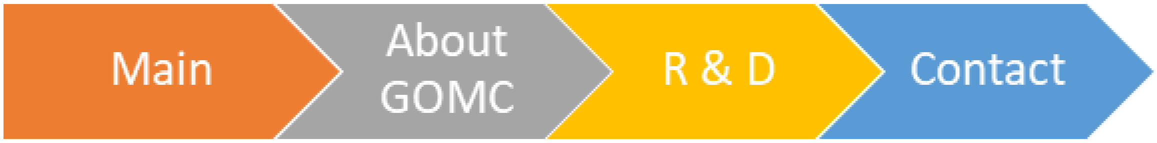
- Grants
- People
- Help

Menu Designs

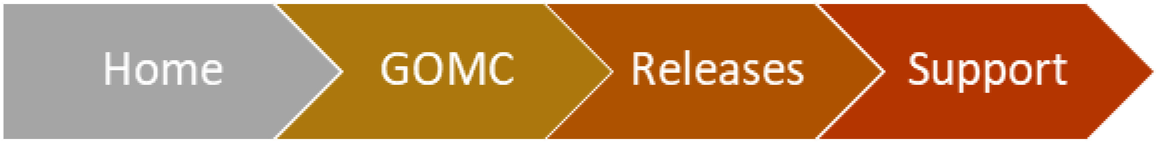
Original



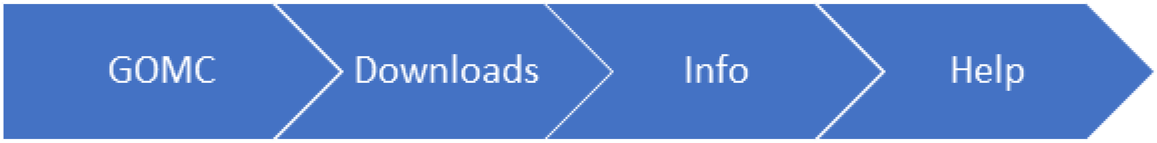
Design 1



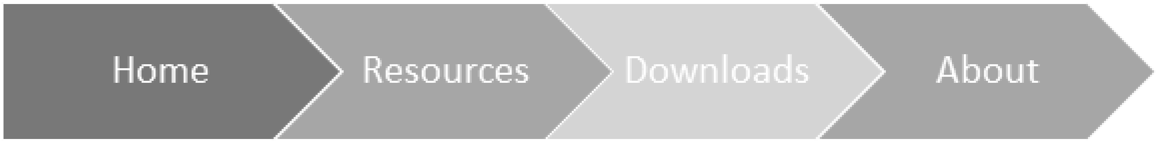
Design 2



Design 3



Design 4

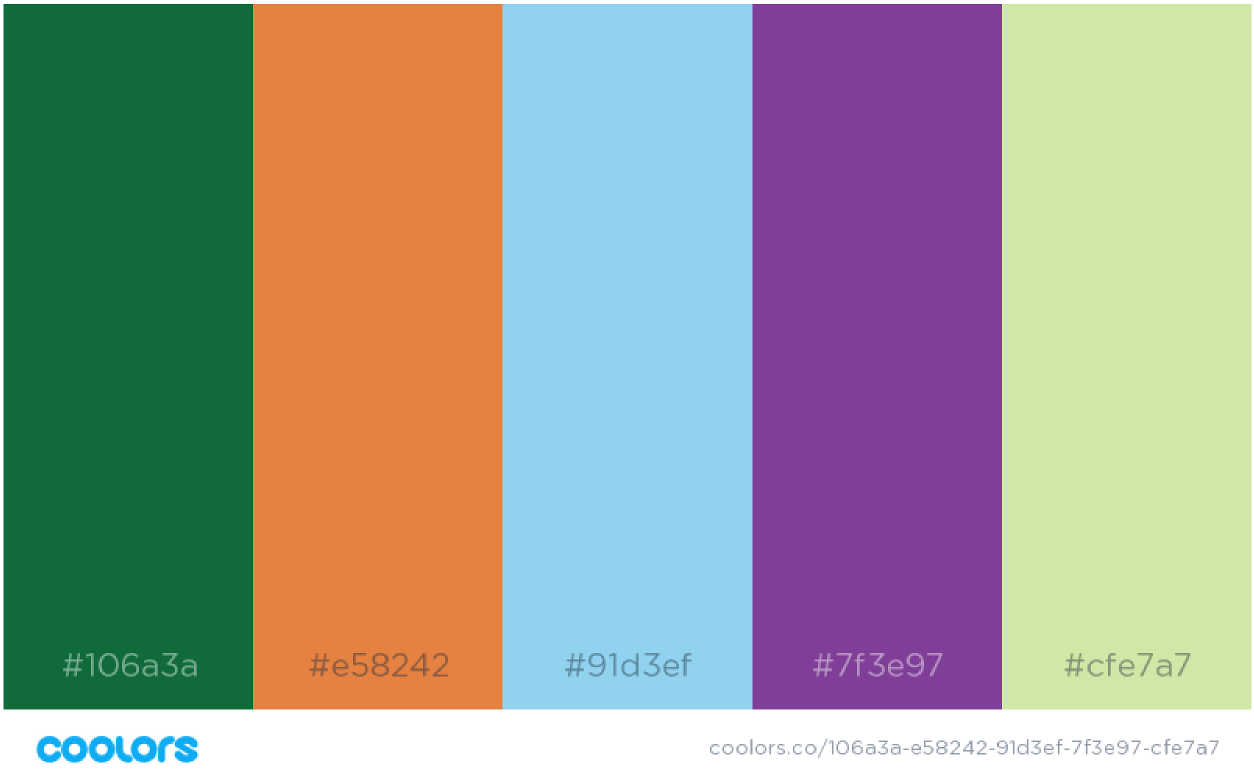


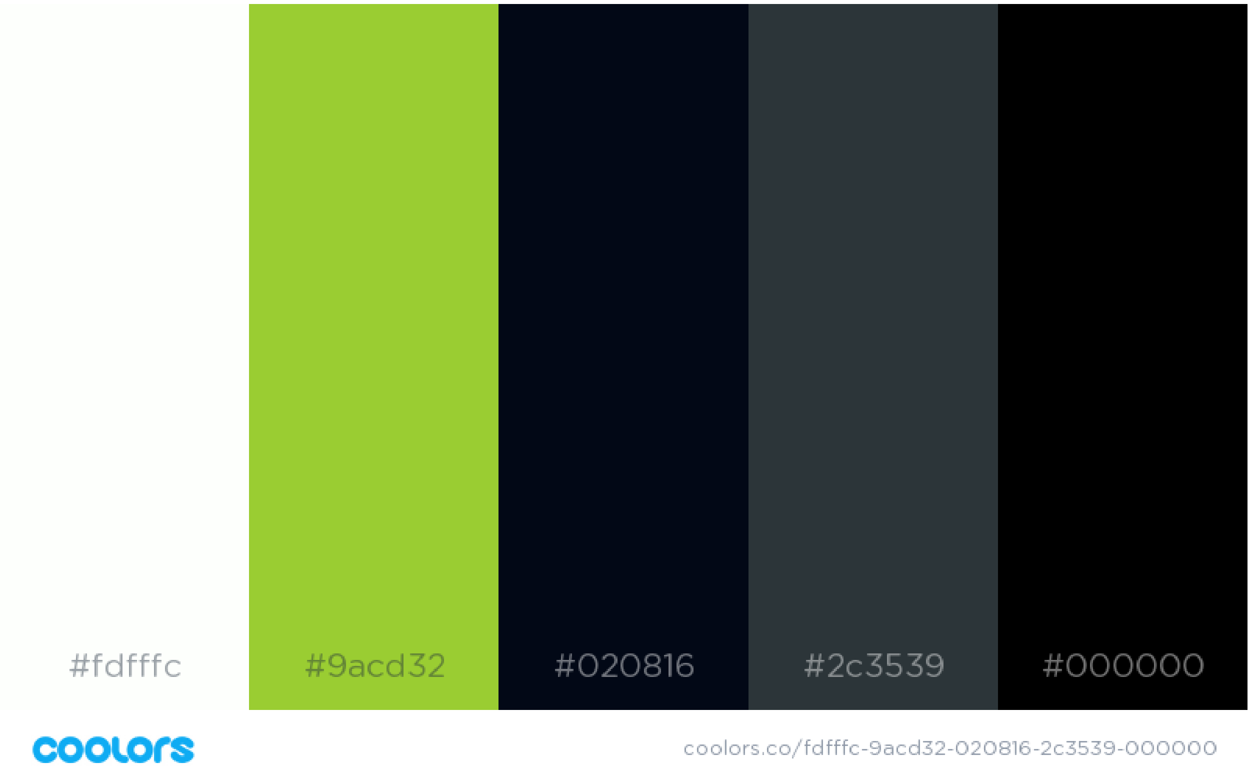
Official colors, Font, and Menu Scheme

In this section the selected colors, fonts and menu scheme have been discussed and agreed upon by the client.

Color Palette

The color palette has two parts the first image will be used for in focus segments of the site. The term “in focused” refers to hover and selection events which will be refined and reviewed with successive UVs. The second is the current color scheme for the site. The background will alternate between “yellow green” and white for different areas. Text will conversely alternate as well to enhance readability.





Font Scheme

After discussion of multiple fonts, the decision was made by our client to go with Roboto for large text such as titles, headers and bold text. With Open Sans as the font for supporting text such as paragraphs and lists.

Below is a text sample of our new font scheme **NOTE this may not render properly if Roboto and open sans are not included please view in google docs with the fonts installed:**

This card has a Roboto Header with an Open Sans Paragraph

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Wings of light and dark spread afar

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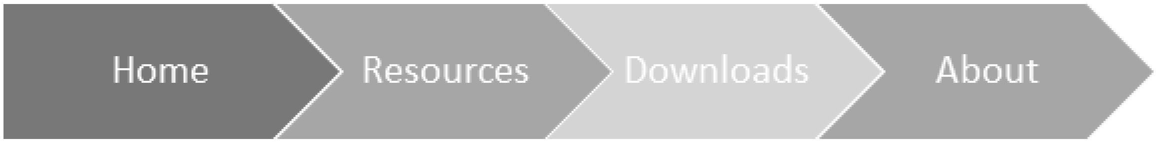
Act III

My friend, do you fly away now?
To a world that abhors you and me?
All that awaits you is a somber morrow
No matter where the winds may blow
My friend, your desire
Is the bringer of life, the gift of the goddess?
Even if the morrow is barren of promises
Nothing shall forestall my return

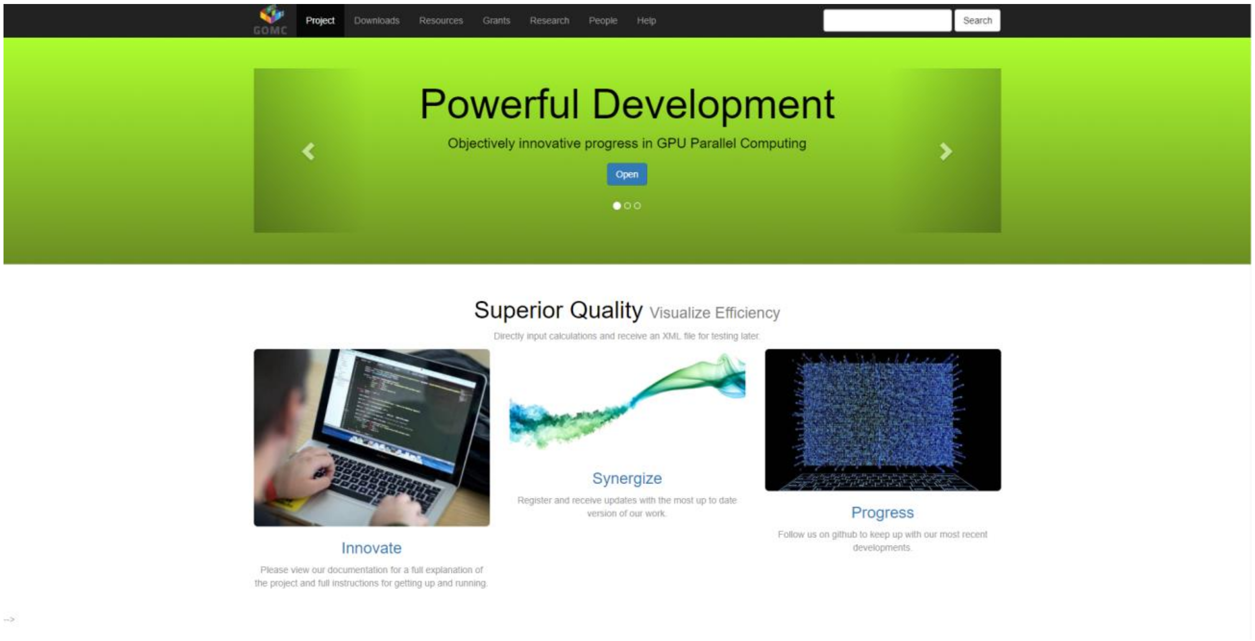
Navbar final

Our navigation bar is still a point of discussion as our clients expressed conflicting views about the navbar selection given how the content is currently expected to be linked. Currently the below is our working version. This may be refined over the course of the next couple of meetings but we expect it will be set in stone by the end of the month.



Other Mockups

Mockup 3



Powerful Development

Objectively innovative progress in GPU Parallel Computing

Superior Quality Visualize Efficiency

Directly input calculations and receive an XML file for testing later.

Innovate

Please view our documentation for a full explanation of the project and full instructions for getting up and running.

Synergize

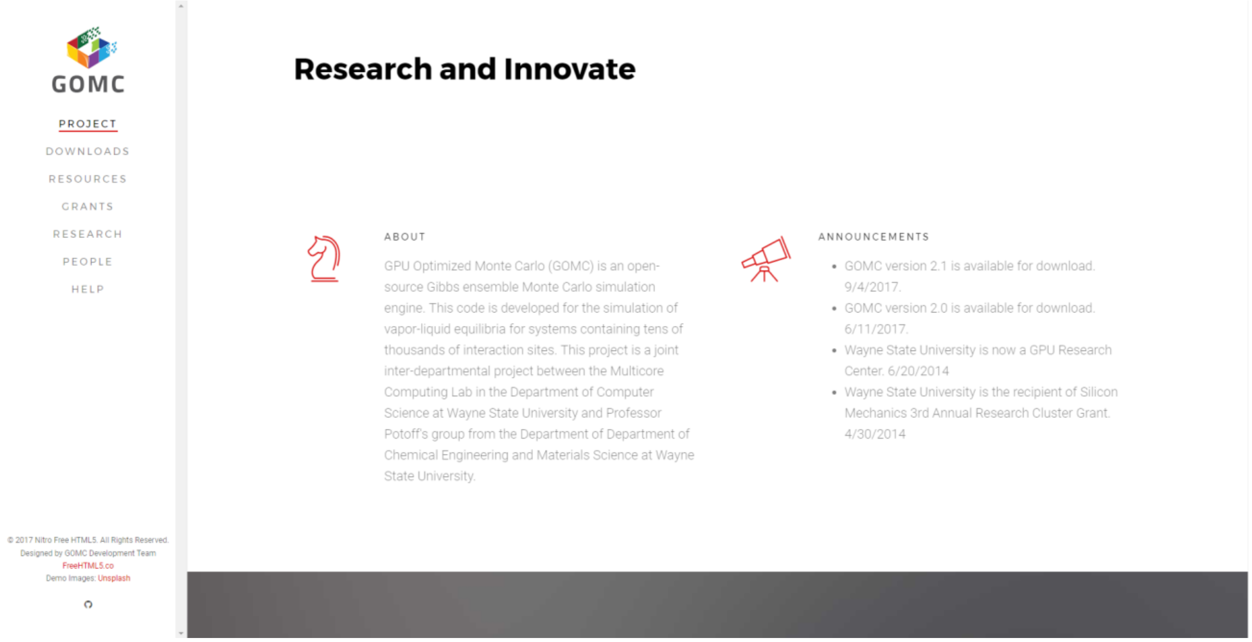
Register and receive updates with the most up to date version of our work.

Progress

Follow us on github to keep up with our most recent developments.

-->

Mockup 4



Research and Innovate

ABOUT

GPU Optimized Monte Carlo (GOMC) is an open-source Gibbs ensemble Monte Carlo simulation engine. This code is developed for the simulation of vapor-liquid equilibria for systems containing tens of thousands of interaction sites. This project is a joint inter-departmental project between the Multicore Computing Lab in the Department of Computer Science at Wayne State University and Professor Potoff's group from the Department of Department of Chemical Engineering and Materials Science at Wayne State University.

ANNOUNCEMENTS

- GOMC version 2.1 is available for download. 9/4/2017.
- GOMC version 2.0 is available for download. 6/11/2017.
- Wayne State University is now a GPU Research Center. 6/20/2014
- Wayne State University is the recipient of Silicon Mechanics 3rd Annual Research Cluster Grant. 4/30/2014

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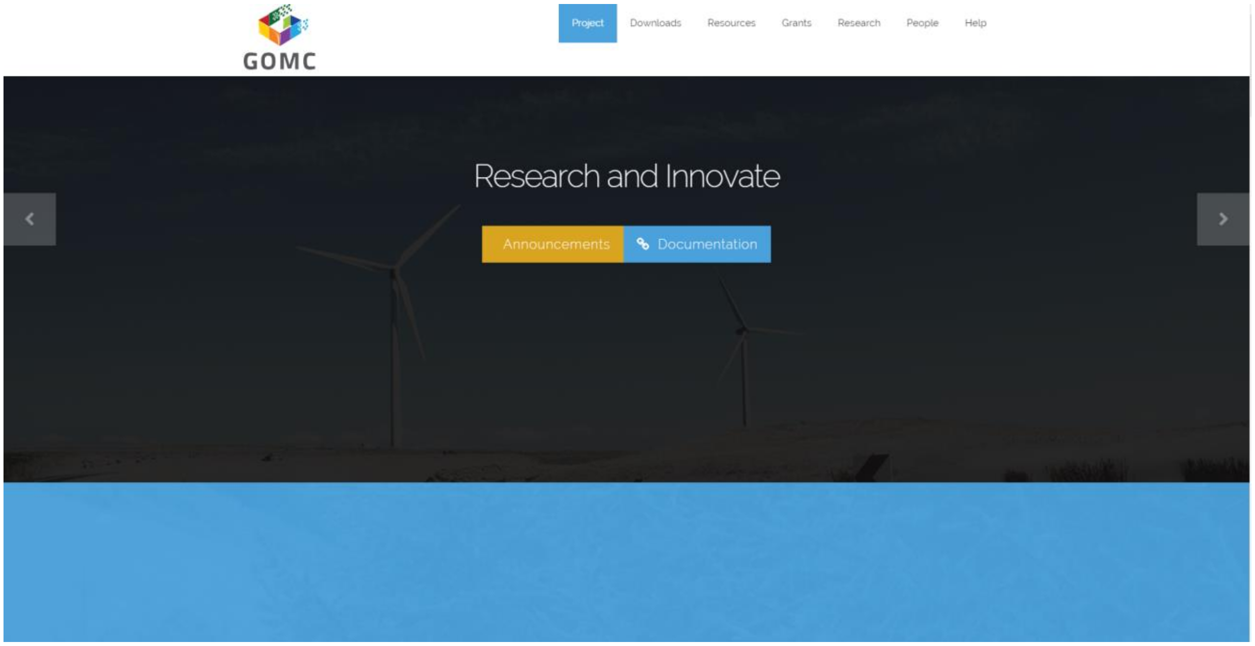
Designed by GOMC Development Team
FreeHTML5.co
Demo Images: Unsplash

Mockup 6



Requirements Traceability Matrix

ID	Related ID	Priority	Title
3.2.1.1	null	1	Downloads Page
3.2.1.2	3.2.1.1	2	Github API Releases
3.2.1.3	3.2.1.2	2	Accept Github Response
3.2.1.4	3.2.1.3	3	Parse JSON
3.2.1.5	3.2.1.4	2	Create Downloads Model
3.2.1.6	3.2.1.1	1	Display Downloads
3.2.2.1	null	1	Input Generator
3.2.2.2	3.2.2.1	1	Download Config XML
3.2.2.3	3.2.2.2	1	Validation
3.2.2.4	3.2.2.3	2	Integer Validation

3.2.2.5	3.2.2.3	2	Float Validation
3.2.2.6	3.2.2.1	2	Enum Fields
3.2.2.7	3.2.2.6	2	Enum Radio
3.2.2.8	3.2.2.6	4	Radio Label
3.2.2.9	3.2.2.3	2	Number Value
3.2.2.10	3.2.2.1	3	Field Label
3.2.2.11	3.2.2.10	3	Field Popup
3.2.2.12	3.2.2.2	2	Download XML button
3.2.3.1	null	1	Login Authentication
3.2.3.2	3.2.3.1	2	Registration
3.2.3.3	3.2.3.2	2	Register with Email
3.2.3.4	3.2.3.2	2	Register with Password
3.2.3.5	3.2.3.2	1	Email Register Valid
3.2.3.6	3.2.3.1	3	Email Login
3.2.3.7	3.2.3.1	3	Password Login
3.2.3.8	3.2.3.1	1	Valid Email Authentication
3.2.3.9	3.2.3.8	1	Valid Password Authentication
3.2.4.1	null	1	Admin View
3.2.4.2	3.2.4.1	1	Authentication
3.2.4.3	3.2.4.2	1	Authorization
3.2.4.4	3.2.4.2	3	Sign-In Request
3.2.4.5	3.2.4.3	3	Invalid Authorization
3.2.4.6	3.2.4.1	1	Number of Downloads

3.2.4.7	3.2.4.1	2	Number of CPU based Apps
3.2.4.8	3.2.4.7	2	Number of GPU based Apps
3.2.4.9	3.2.4.1	2	Number of Windows based Apps
3.2.4.10	3.2.4.1	2	Number of Linux based Apps
3.2.4.11	3.2.4.1	2	Number of Mac based Apps
3.2.4.12	3.2.4.1	2	Number of NVT based Apps
3.2.4.13	3.2.4.1	2	Number of NPT based Apps
3.2.4.14	3.2.4.1	2	Number of NVT Gibbs based Apps
3.2.4.15	3.2.4.1	2	Number of NPT Gibbs based Apps
3.3.4.16	3.2.6.1	2	LaTeX Upload
3.2.5.1	null	1	Parse
3.2.5.2	3.2.5.1	2	Validation
3.2.5.3	3.2.5.2	2	Valid XML
3.2.5.4	3.2.5.2	2	XML Schema Validation
3.2.5.5	3.2.5.3	3	Parse Fail Handling
3.2.5.6	3.2.5.4	3	Invalid Schema Handling
3.2.5.7	3.2.5.1	3	Error Output
3.2.6.1	null	1	Conversion
3.2.6.2	3.2.6.1	2	HTML sections

3.2.6.3	3.2.6.2	3	HTML Links
3.2.6.4	3.2.6.1	2	Search
3.2.6.5	3.2.6.4	3	Search List Results
3.2.6.6	3.2.6.5	2	Search Results Item
3.2.6.7	3.2.6.3	2	PDF Links
3.2.6.8	3.2.6.1	3	PDF Download
3.3.1.1	null	2	Page Load Time
3.3.1.2	null	1	Web Site Storage
3.3.1.3	null	1	Web Site Ram
3.3.1.4	null	2	User Count
3.3.2.1	3.3.3.1	2	Downtime
3.3.2.2	null	3	Bug Count
3.3.3.1	null	1	Availability
3.3.3.2	3.3.3.2	4	Maintenance
3.3.4.1	null	1	Enforce Security Standards
3.3.4.2	3.3.4.1	1	Authentication for Admin Page
3.3.4.3	3.3.4.2	2	Authorization for Admin Page
3.3.4.4	3.3.4.1	1	Passwords Hashed

Terms table

Below is a full table of all the terms and acronyms used by the dev-team over the course of this project and their meanings. You can find a shorter excerpt of this table that more strongly correlates to this document in section 1.3.

Term	Meaning
UI	User Interaction
UX	User Experience
JS	JavaScript
VMD	Visual Molecular Dynamics
VLE	Saturated Vapor-Liquid Equilibria
MC	Markov Chain
Boltzmann	Boltzmann Sampling
Priority	The measure of importance of a requirement, i.e., priority 1 is more important (higher priority) than priority 2
GOMC	GPU-Optimized Monte-Carlo simulation engine
GOMC Research	The team that our client is a part of. The development and research of the engine and molecular structures, systems and ensembles that it supports
Check in	Committing and Pushing new code or other files to our remote repo
Commit	Staging changes, with a message explaining what the changes entail

Push	Sending new commits to the remote repo
Merge	Perform a code review on a pull request and combine the changes in with the branch
Branch	A copy of the repo with modifications for a specific feature
Repo	A folder stored in a remote location for development purposes. Serves as a medium for collaboration.
Clone	Making a copy of a repo on a local computer for development.
Pull	Pull Request, propose changes for a feature branch. Submitting this means that a developer is ready for their work to be reviewed and if approved become part of the application
WFH	Work from home on a desktop environment
WFR	Work from remote on a laptop environment
CWFH	Checking in to work from home, seeing this in a commit message indicates that the developer is checking in their work to pull-latest on their desktop to continue work. This kind of commit indicates that work is only being moved and that it’s not done yet.
CWFR	Checking in to work from remote, seeing this in a commit message indicates that the developer is only checking in to pull-latest on their laptop and continue work. This kind of commit indicates that work is only being moved and that it’s not done yet.

Pull-Latest	Pulling latest, grabbing latest or fetching latest all refer to grabbing the latest version of a branch on the repo
API	Application programming interface, in our case we will be referring to the github API v3
Underscore	Underscore.js is a very popular library of JavaScript and a source of a lot of functionality
Less	Less.css is a compiled form of CSS that allows a developer to write and port modules. Less will refer to these modules and their functionality
Standup	A daily report in our slack chat detailing what you did yesterday, what you are working on today and if you need support from anyone
UV	A demo to the client of some feature or design that they can give verbal feedback on. Also referred to as demos or client presentations
Beta	Our lower environment
Master	Our main environment
Downloads	A core feature of the downloads page using the github API
XML file	A core feature of taking form data, generating an xml file and sending that to an endpoint
Admin-Dash	A core feature of the admin dashboard

Doc-viewer	A core feature of converting and reading documents in html
P11 P12 and p2	Prototype 1-1, Prototype 1-2 and prototype 2
Gulp	Gulp.js is an automated task runner for making builds. It is part of our test suite
Site	When we say site, app or product we are talking about the whole summation of the deliverables
Ensemble	Structure and context of molecules
GOMC Dev-Team	The development team for this project
S1 - S7	Referring to screens 1- 7 of the of the current website
Enum	An enumerated type in a programming language which is a set of named values.
Distribution or dist/	A minified, uncommented version of a set of files. JavaScript files concatenated into a single file. Minimized for minimal bloat on client server and optimized for speed. This version of the code base runs in the production environment. It lives on our master branch in the repo and on our main server.
Source or src/	A development version of the code base. The exact opposite of the Distribution, lives on local. Changes to the code base are done to source first. Source is compiled, linted, validated, minified and tested before producing distribution. Source lives on our

	dev server and in our beta branch.
Master Server	Server supporting the website linked at the gomc.eng.wayne.edu space. Viewable by client and users.
Dev Server	Internal server for the team with code integrated from the beta branch. Can be found at ahtaher.net
Config Page	Also known as Config input page. This page is used for allowing the user to input config fields and then downloading the result as an XML file.