Version Control Workshop: Git and GitHub (Day 2)

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GitHub



Overview

- GitHub Pages and Jekyll
- Q GitHub Mobile App
- GitHub Student Developer Pack
- 4 GitHub Community
- 6 Programming Challenges



Pages

- GitHub allow users to have one personal (static) site.
- 2 It also allows one site per project.
- 3 Jekyll is the site-generator behind GitHub Pages.



Mobile App





Mac



It is not a replacement for a desktop client, but it is good enough to keep track of some changes on the go.



GitHub Pages

A couple of months ago GitHub (with some companies) released a pack of free tools for students:

https://education.github.com/pack



GitHub Student Developer Pack

- **4 Atom:** A text editor developed by GitHub

- SendGrid: Email services



GitHub Pages

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GitHub Open Source Projects

Some major open source projects include:

- **Jekyll:** https://github.com/jekyll/jekyll
- Linux Kernel: https://github.com/torvalds/linux
- Matplotlib: https://github.com/matplotlib/matplotlib
- Ruby on Rails: https://github.com/rails/rails
- Scipy Lecture Notes: https://github.com/scipy-lectures/scipy-lecture-notes



More Cool Projects

- D3: https://github.com/mbostock/d3
- Flatland A Romance of Many Dimensions: https://github.com/Ivesvdf/flatland
- Generate DOI for Github Repos: https: //guides.github.com/activities/citable-code/
- GitBook (Books Editor): https://www.gitbook.io/
- GitHub Visualizer: http://ghv.artzub.com/
- ShareLatex: https://github.com/sharelatex/sharelatex



GitHub Pages

- Choosing an OSS License: http://choosealicense.com/
- GitHub Explore: https://github.com/trending
- Gitter: https://gitter.im
- LearnProgramming:

http://learnprogramming.github.io/



Verlet Integration

- Verlet integration is a numerical method used to integrate Newton's equations of motion.
- It is frequently used to calculate trajectories of particles in molecular dynamics simulations and computer graphics.



GitHub Pages

• If we do a Taylor expansion of the position vector $\vec{x}(t \pm \Delta t)$ forwards and backward we get:

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\Delta t + \frac{\vec{a}(t)\Delta t^2}{2} + \frac{\vec{b}(t)\Delta t^3}{6} + \mathcal{O}(\Delta t^4)$$
$$\vec{x}(t-\Delta t) = \vec{x}(t) - \vec{v}(t)\Delta t + \frac{\vec{a}(t)\Delta t^2}{2} - \frac{\vec{b}(t)\Delta t^3}{6} + \mathcal{O}(\Delta t^4),$$



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Adding these two expansions gives:

$$\vec{x}(t + \Delta t) = 2\vec{x}(t) - \vec{x}(t - \Delta t) + \vec{a}(t)\Delta t^2 + \mathcal{O}(\Delta t^4).$$

We can see that the first and third-order terms from the Taylor expansion cancel out, thus making the Verlet integrator an order more accurate than integration by simple Taylor expansion alone.

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So we can use as time stepper the equation

$$\vec{x}(t + \Delta t) = 2\vec{x}(t) - \vec{x}(t - \Delta t) + \vec{a}(t)\Delta t^{2},$$

or in terms of forces

$$\left| \vec{x}(t + \Delta t) = 2\vec{x}(t) - \vec{x}(t - \Delta t) + \frac{\vec{F}(t)}{m} \Delta t^2 \right|,$$



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Our goal is to create a solver for Newton equations using Verlet integration. We can split the project into small groups.

A possible division of labors is:

- Force Routines (Springs, Electrostatic Interactions, etc.)
- Verlet Step Calculator for Different Coordinates (x, y, z)
- Verlet Time Stepper:
- Plotting Capabilities
- Main Routines



Programming Challenges

 We have a set of simple programming challenges stored in the programming_challenges directory of the main repo.

GitHub Community

- Try to commit your code in three ways:
 - Locally on your computer
 - Remotely on your GitHub account
 - Via pull request on Cyrus' GitHub account

