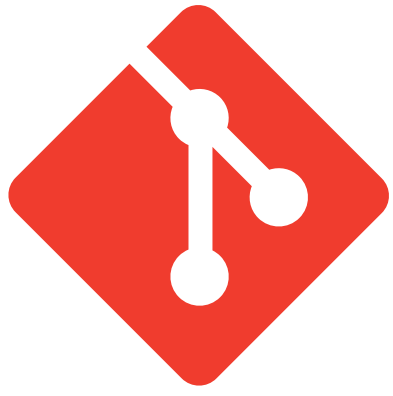
PURDUE
UNIVERSITY

Day 2

Workshop: Git and GitHub



git

Cyrus Vandrevala [1]
Nicolás Guarín-Zapata[2]
[1] Physics Department
[2] Civil Engineering Department
October 28, 2014

Overview

1. GitHub Pages and Jekyll
2. GitHub Mobile App
3. GitHub Student Developer Pack (GitHub Education)
4. GitHub Open Source Projects
5. GitHub Community
6. Programming Example
7. Programming Challenges

Disclaimer

Pages

1. GitHub allow users to have one personal (static) site.
2. Allows a site per project.
3. Jekyll is the site-generator behind GitHub Pages. There are plenty of templates written in Liquid. [1]

[1] See here `http://jekyllrb.com/docs/templates/`. If you are one of those geeks... you can also use CSS templates.

Pages

1. GitHub allow users to have one personal (static) site.
2. Allows a site per project.
3. Jekyll is the site-generator behind GitHub Pages. There are plenty of templates written in Liquid. [1]

[1] See here `http://jekyllrb.com/docs/templates/`. If you are one of those geeks... you can also use CSS templates.

Pages

1. GitHub allow users to have one personal (static) site.
2. Allows a site per project.
3. Jekyll is the site-generator behind GitHub Pages. There are plenty of templates written in Liquid. [1]

[1] See here `http://jekyllrb.com/docs/templates/`. If you are one of those geeks... you can also use CSS templates.

Mobile App

GitHub for Android[a]

1. Issue Dashboard.
2. Gist Support.
3. News Feed.

[a] https://mobile.github.com/

Off course, it is not a replacement for a Desktop client. But it is good enough to keep track of some changes on the go.

GitHub Student Developer Pack

A couple of months ago GitHub (with some companies) released a pack of free tools for students[2]. Here we present some of them that were arbitrarily chosen.

1. Atom: a text editor developed by GitHub.
2. CrowdFlower: data enrichment, data mining and crowdsourcing services.
3. GitHub: 5 Private GitHub Repos.
4. SendGrid: Email services.
5. Unreal Engine: A suite of game development tools for PC, console, mobile and web.

[2] https://education.github.com/pack

GitHub Student Developer Pack

A couple of months ago GitHub (with some companies) released a pack of free tools for students[2]. Here we present some of them that were arbitrarily chosen.

1. Atom: a text editor developed by GitHub.
2. CrowdFlower: data enrichment, data mining and crowdsourcing services.
3. GitHub: 5 Private GitHub Repos.
4. SendGrid: Email services.
5. Unreal Engine: A suite of game development tools for PC, console, mobile and web.

[2] https://education.github.com/pack

GitHub Student Developer Pack

A couple of months ago GitHub (with some companies) released a pack of free tools for students[2]. Here we present some of them that were arbitrarily chosen.

1. Atom: a text editor developed by GitHub.
2. CrowdFlower: data enrichment, data mining and crowdsourcing services.
3. GitHub: 5 Private GitHub Repos.
4. SendGrid: Email services.
5. Unreal Engine: A suite of game development tools for PC, console, mobile and web.

[2] https://education.github.com/pack

GitHub Student Developer Pack

A couple of months ago GitHub (with some companies) released a pack of free tools for students[2]. Here we present some of them that were arbitrarily chosen.

1. Atom: a text editor developed by GitHub.
2. CrowdFlower: data enrichment, data mining and crowdsourcing services.
3. GitHub: 5 Private GitHub Repos.
4. SendGrid: Email services.
5. Unreal Engine: A suite of game development tools for PC, console, mobile and web.

[2] https://education.github.com/pack

GitHub Student Developer Pack

A couple of months ago GitHub (with some companies) released a pack of free tools for students[2]. Here we present some of them that were arbitrarily chosen.

1. Atom: a text editor developed by GitHub.
2. CrowdFlower: data enrichment, data mining and crowdsourcing services.
3. GitHub: 5 Private GitHub Repos.
4. SendGrid: Email services.
5. Unreal Engine: A suite of game development tools for PC, console, mobile and web.

[2] https://education.github.com/pack

GitHub Open Source Projects

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

GitHub Open Source Projects

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

GitHub Open Source Projects

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

GitHub Open Source Projects

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

Cool stuff

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

Cool stuff

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

Cool stuff

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

GitHub Community

- GitHub Explore: https://github.com/trending

GitHub Community

- GitHub Explore: https://github.com/trending

Verlet Integration I

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

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

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

Verlet Integration II

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. So we can use as time stepper the equation

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

or in terms of forces

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

Verlet Integration III

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, some wacky stuff);
- Verlet step calculator for different coordinates x, y and z;
- Verlet time stepper;
- Plotting capabilities; and
- Main routines.

Small programming

We have a set of *simple* programming tasks. The main idea is to get a set of different solutions to compare the execution times or the codes. Please commit your code as `probX_ID.ext`, where `X` is the number of the problem, `ID` and `ext` is the extension of the file.
Add directory to make commits.

Thank you for your attention.