#### Workshop: Git and GitHub (Day 2)

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**GitHub** 



Workshop: Git and GitHub (Day 2)







#### Overview

- GitHub Pages and Jekyll
- Q GitHub Mobile App
- GitHub Student Developer Pack (GitHub Education)
- 4 GitHub Open Source Projects
- 6 GitHub Community
- 6 Programming Example
- Programming Challenges



2014-10-30

└**O**verview

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Overview

GitHub Pages and Jekyll

GitHub Mobile App
GitHub Student Developer Pack (GitHub Education)

GitHub Open Source Projects

GitHub Community

Programming Example

Programming Challenges

- Post Questions That You Might Have in the Repo
- Recommend Other Sources That You Found Useful
- Remember, We Do Not Know Everything!



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#### **Pages**

- 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

<sup>&</sup>lt;sup>1</sup>See here http://jekyllrb.com/docs/templates/. If you are one of those geeks... you can also use CSS templates.



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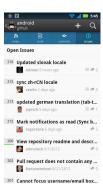
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#### Mobile App

GitHub Pages



GitHub for Android<sup>a</sup>

- Issue Dashboard.
- Gist Support.
- News Feed.

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.



Challenges

ahttps://mobile.github.com/

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GitHub Mobile App

Mobile App

GitHub for Androids

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- SendGrid: Email services.

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Workshop: Git and GitHub (Day 2) └─GitHub Open Source Projects

GitHub Open Source Projects

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- GitHub Visualizer: http://ghv.artzub.com/
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# Verlet Integration I

GitHub Pages

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

GitHub Pages

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

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

or in terms of forces

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



## Verlet Integration III

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



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- Protting capacitors; and
   Main routines.

#### Small programming tasks

GitHub Pages

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. There is a directory named ./programming\_challenges/, where you should commit your solutions.



Thank you for your attention.

