SESSION 2

Hybrid Particle-In-Cell

Particle pusher

GIT: VERSION CONTROL

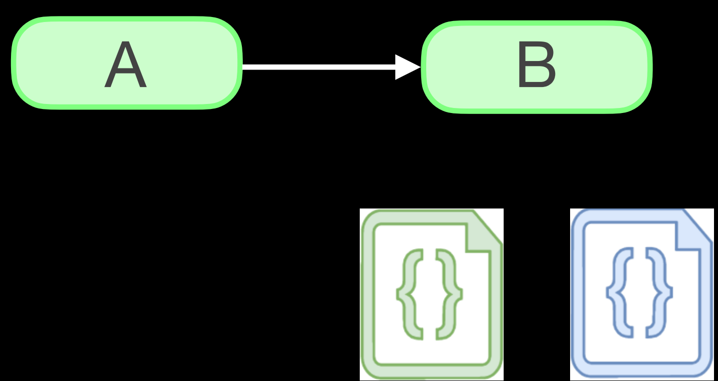
A typical Programming problem

Say you have a directory on which you work…

A

- a.txt
-

You have a.txt and you add b.txt

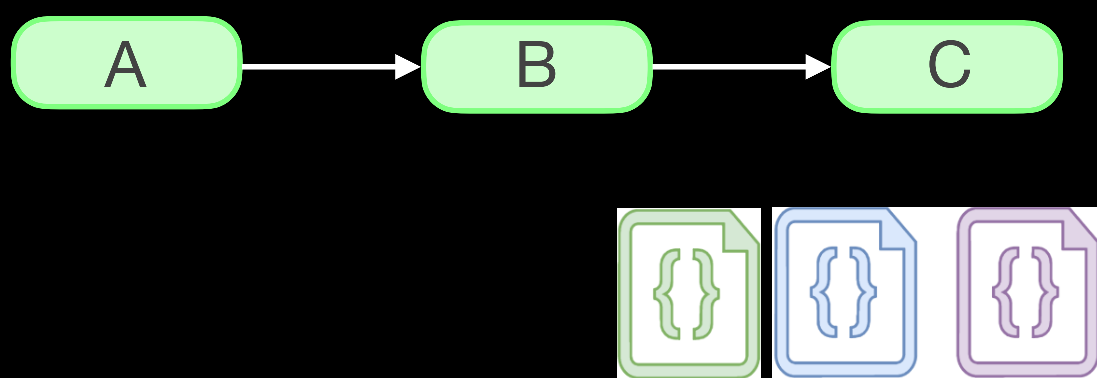


- a.txt
- b.txt

Git in a nutshell

Then you realize there is maybe a better way to write b.txt

You want to write a new version but keep the current in the mean time?

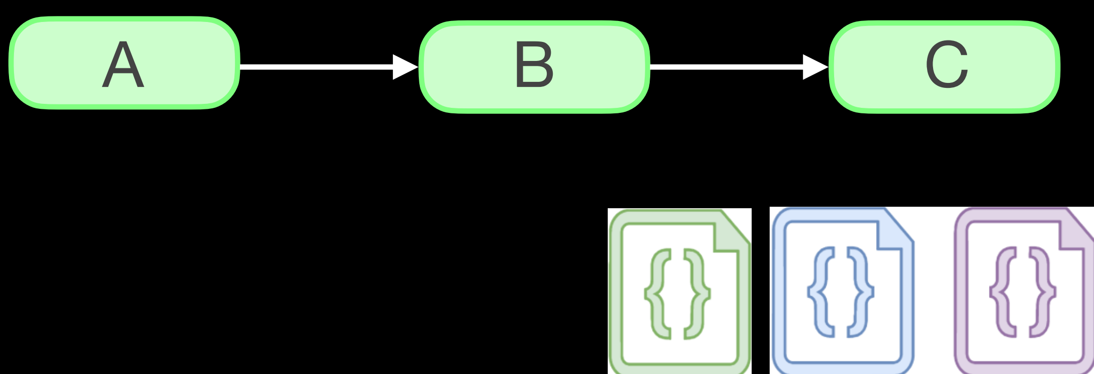


- a.txt
- b.txt
- b-old.txt

Git in a nutshell

Your colleague now tells you you have a bug in a.txt

….



- a.txt
- b.txt
- b-old.txt

6 months later, you start everything all over…

Git in a nutshell

- Official documentation: https://git-scm.com
- play online to learn : https://learngitbranching.js.org/?locale=fr_FR
- Understand git visually: https://marklodato.github.io/visual-git-guide/index-en.html
- Github documentation : https://docs.github.com/fr/get-started/start-your-journey/hello-world

git is a command line software. There are GUI applications wrapping it. But in my opinion you should use them only if you understand git commands first.

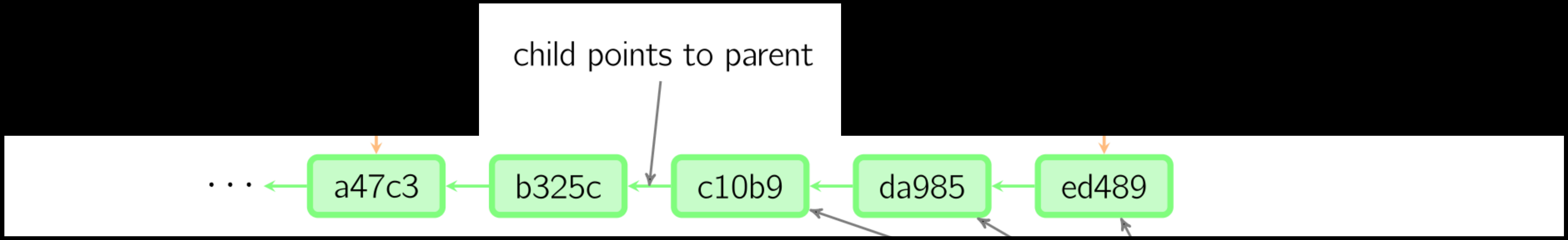
I have used git for 10 years. I by far mostly use:

- Add
- Commit
- Rebase
- Merge
- Push
- Clone

These are « commits », saved states of your code

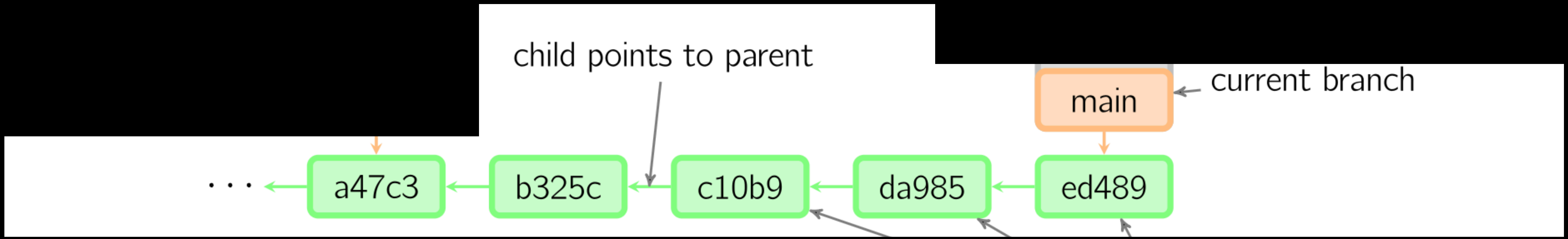
Each commit knows about its parent

A chain of commit is your commit history

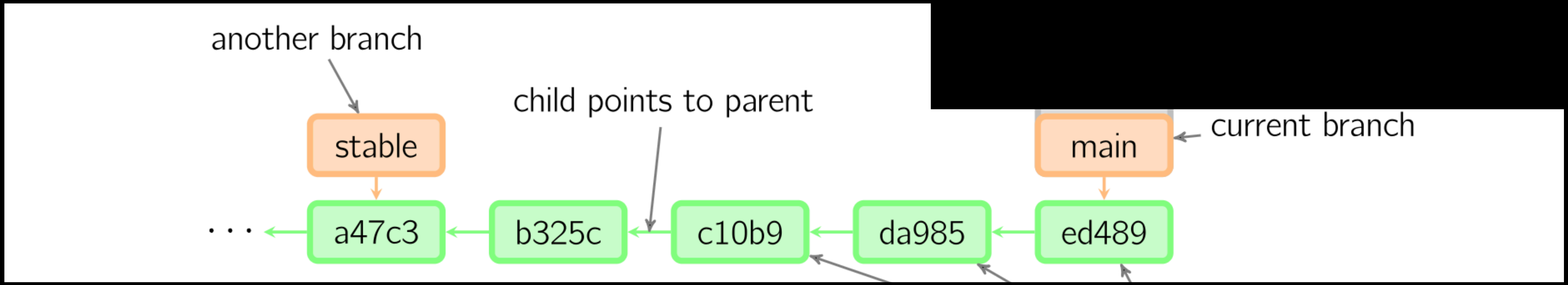


A particular history is called « a branch »

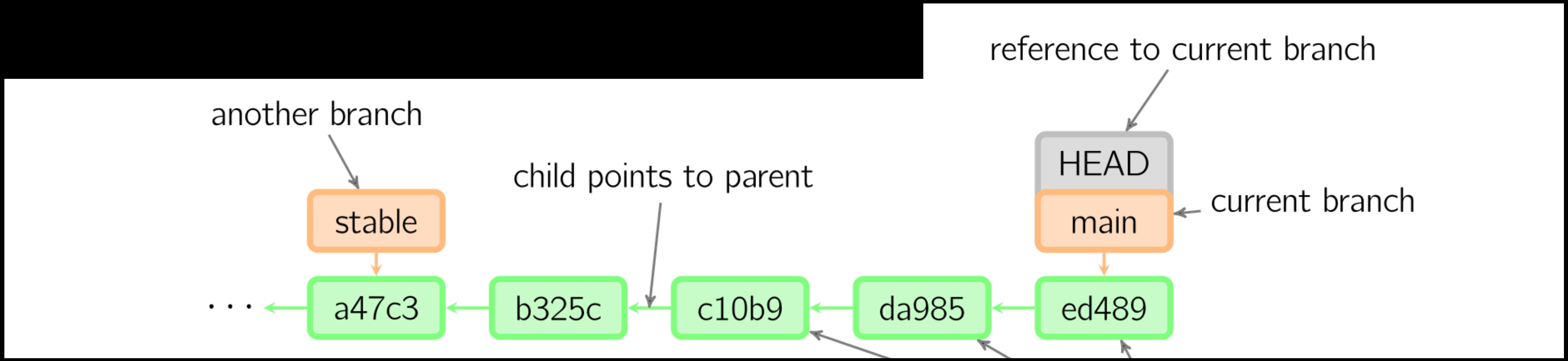
A branch has a name, here « main » (default is « master »)



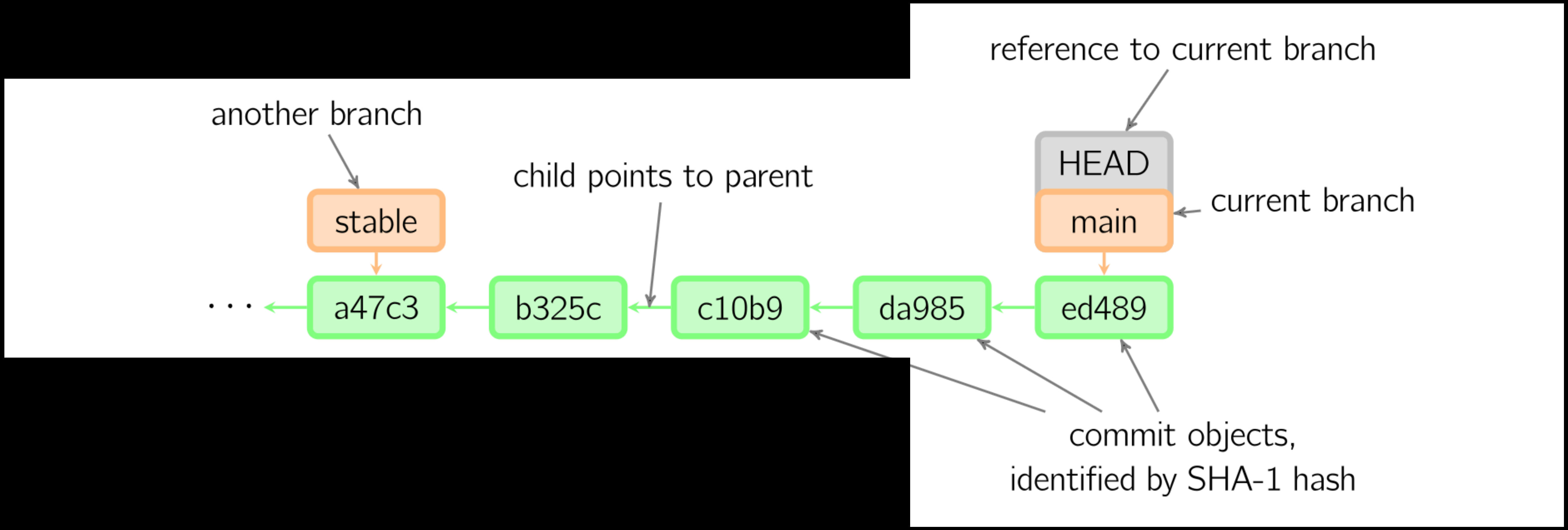
You can have several branches, pointing at different commits, therefore tracking different histories



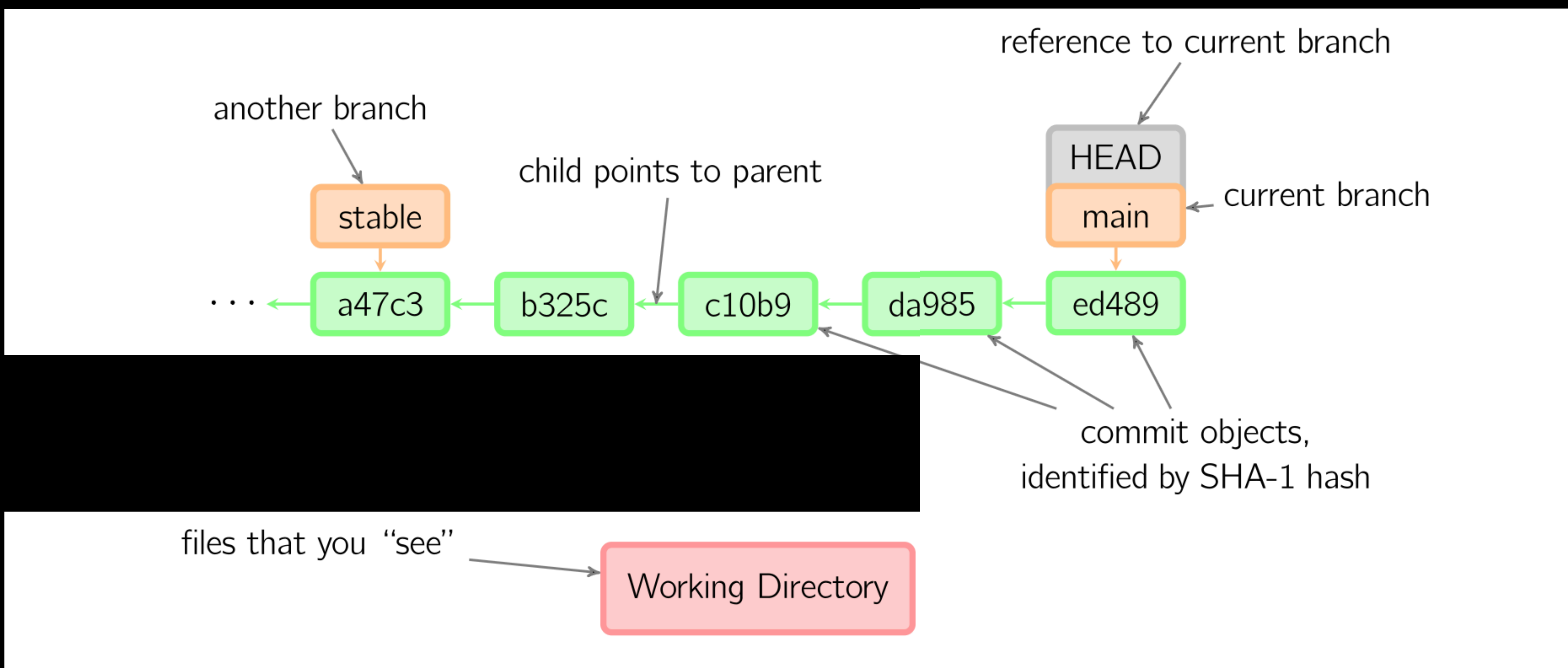
« HEAD » is a reference to where you are at a given time



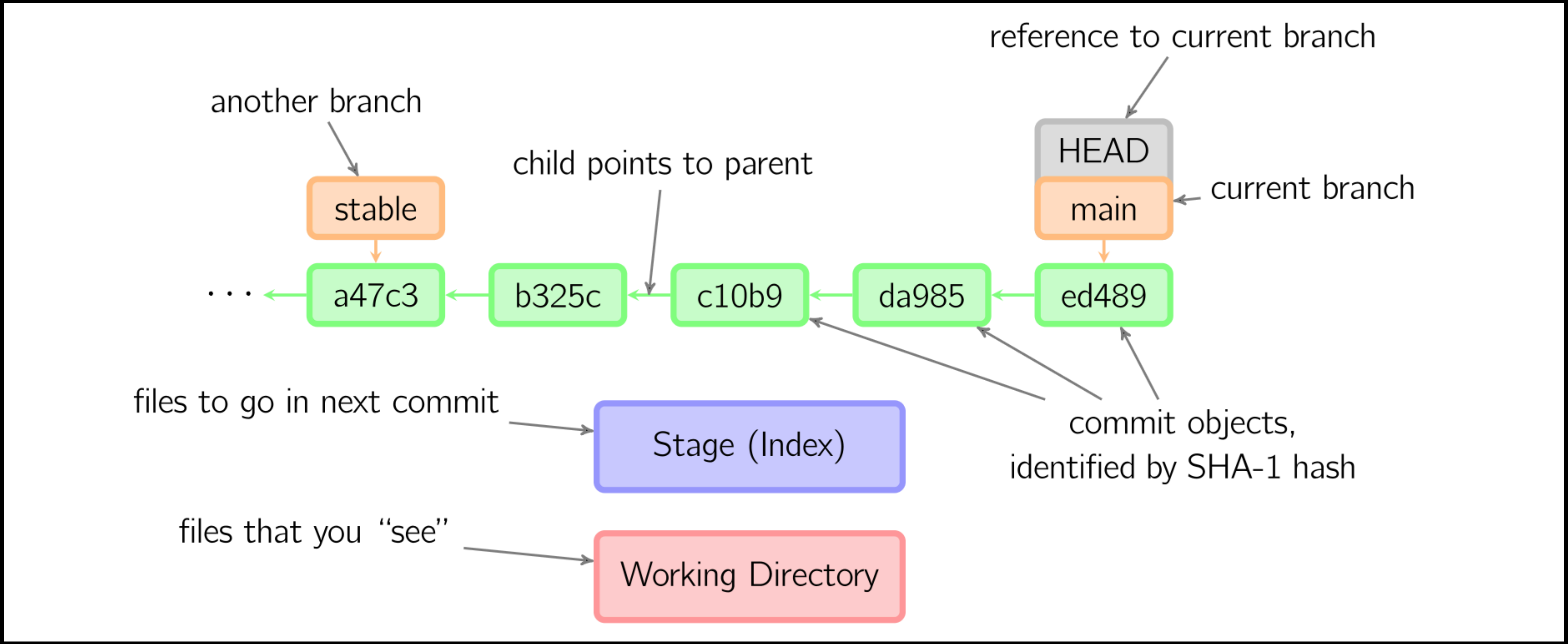
Each commit has unique identifier (called a SHA-1 - Simpler Hashing Algorithm - 1)



Besides the commit history, the files you're working on currently are in the « working directory »

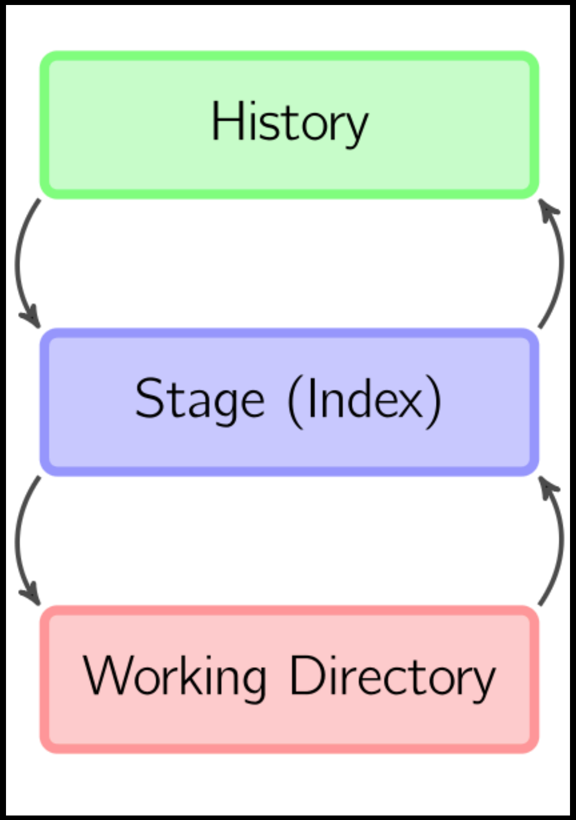


And what is about to be committed is in the « stage »

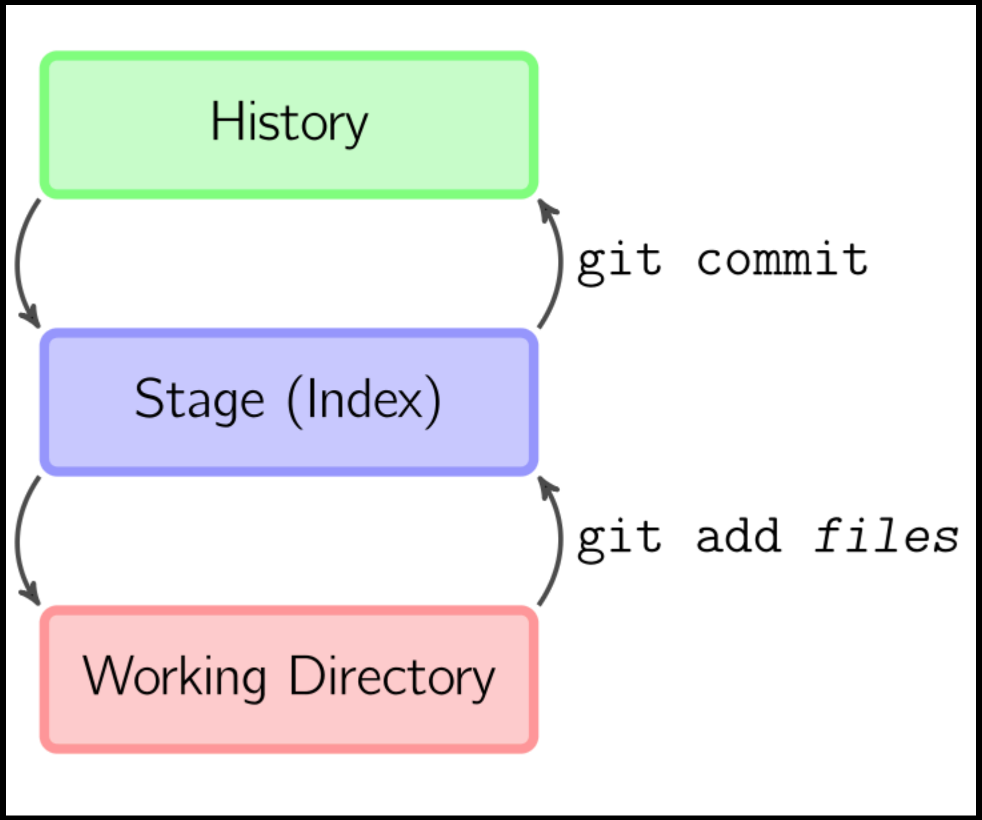


Why a stage?

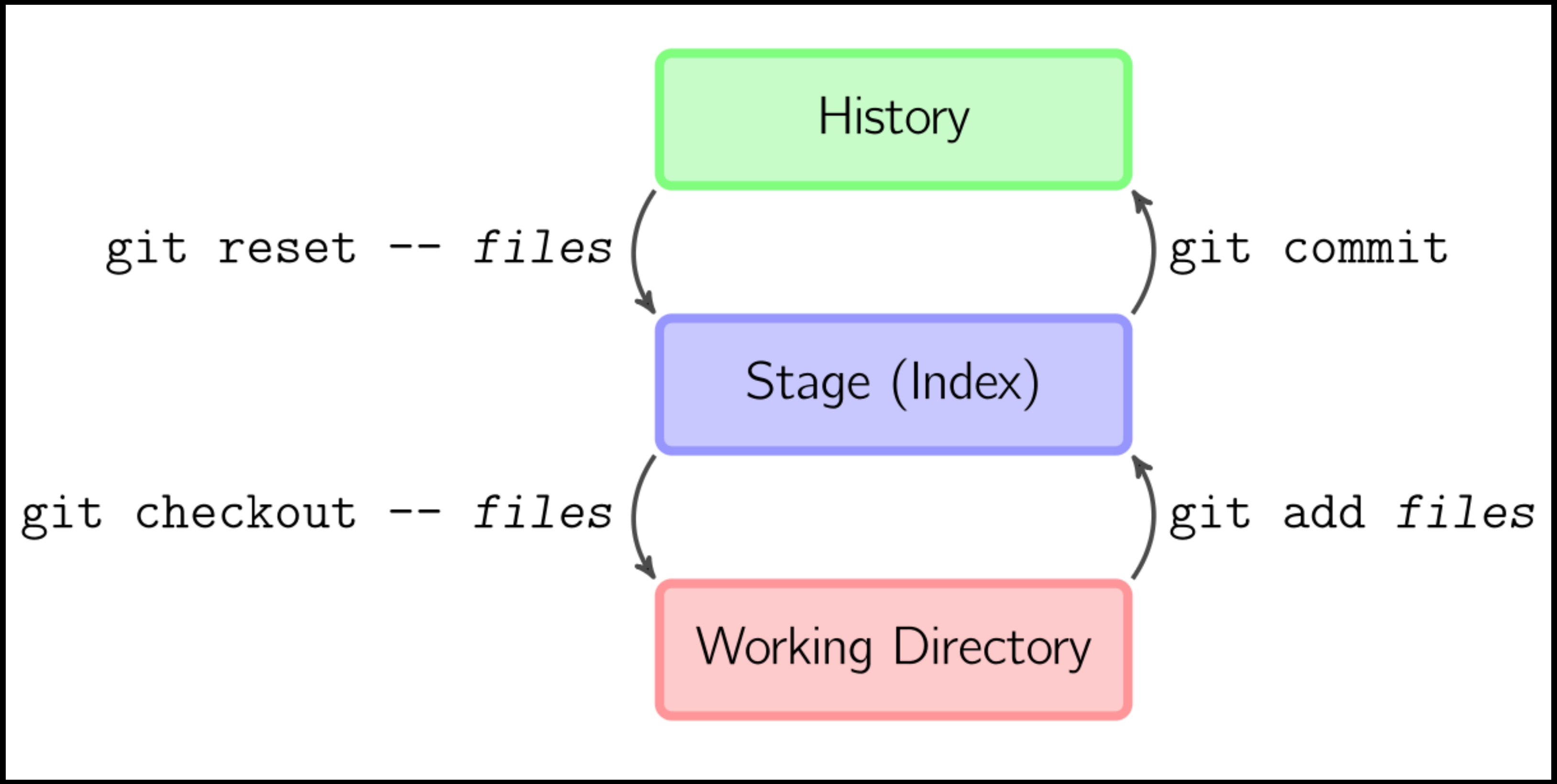
Why a stage?



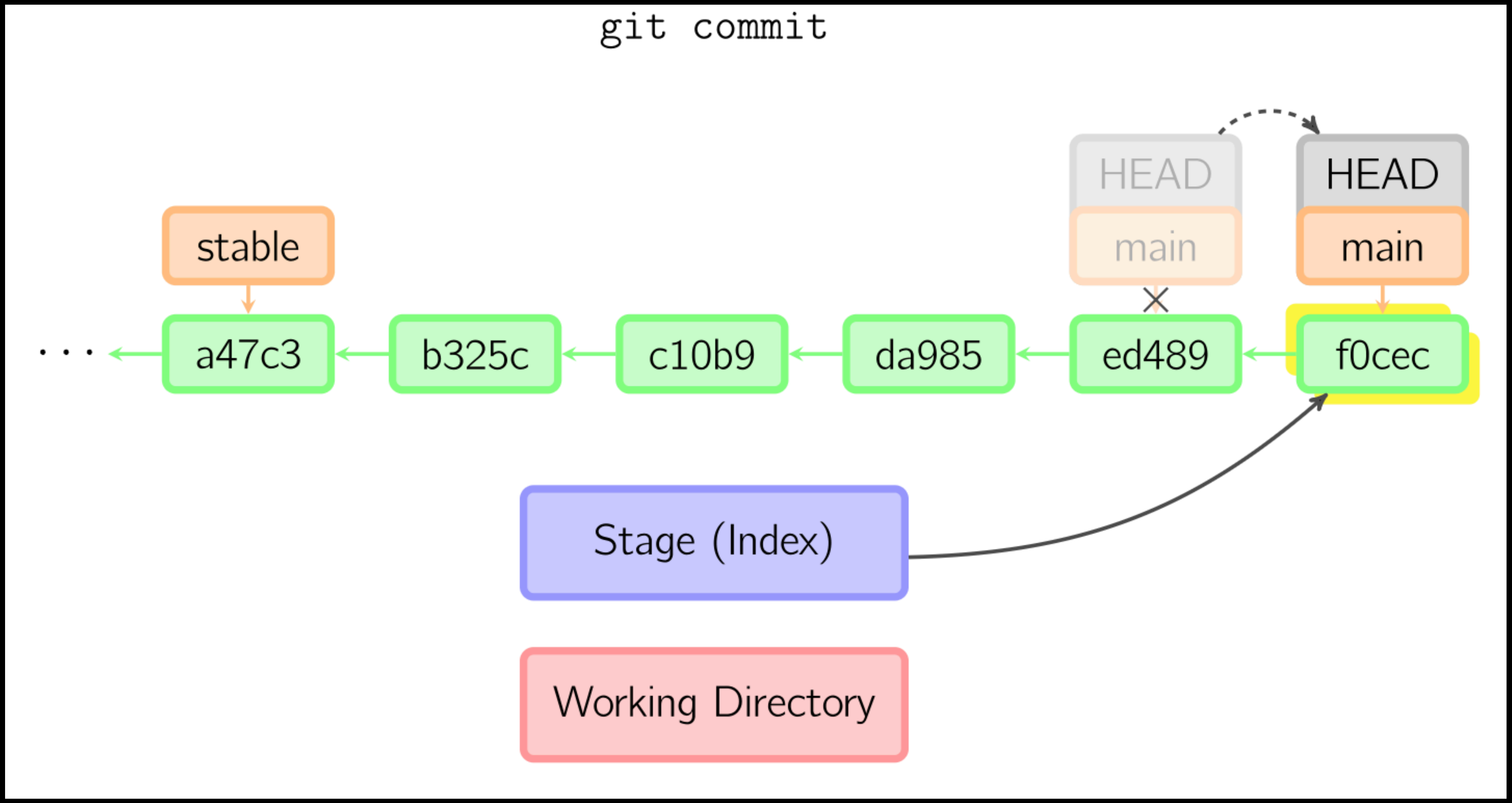
You may not want to commit every change made in the current working directory?



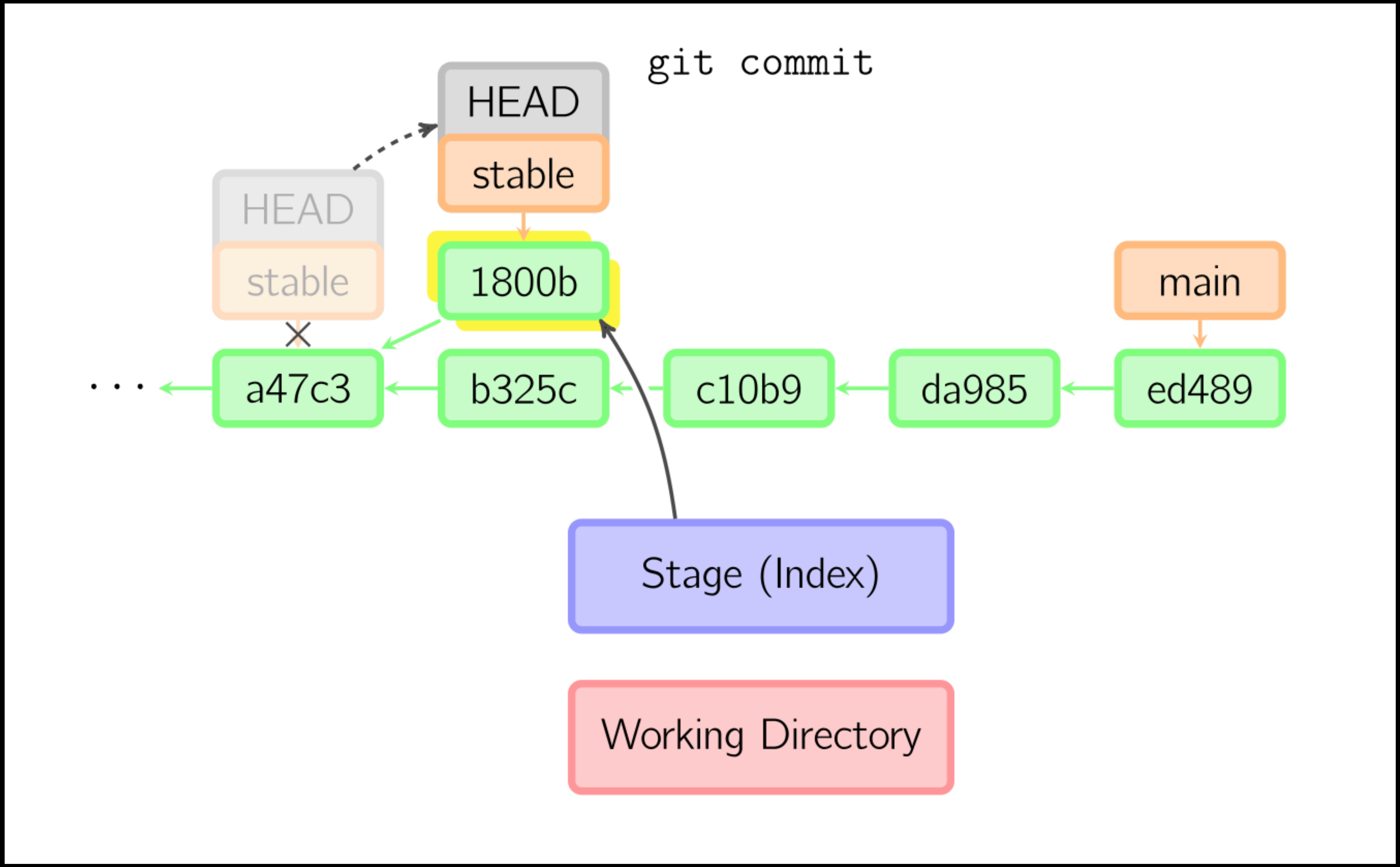
Opposite « motions » are also possible.



A commit is adding the increment from the stage into the history and moving the current branch and HEAD to that commit

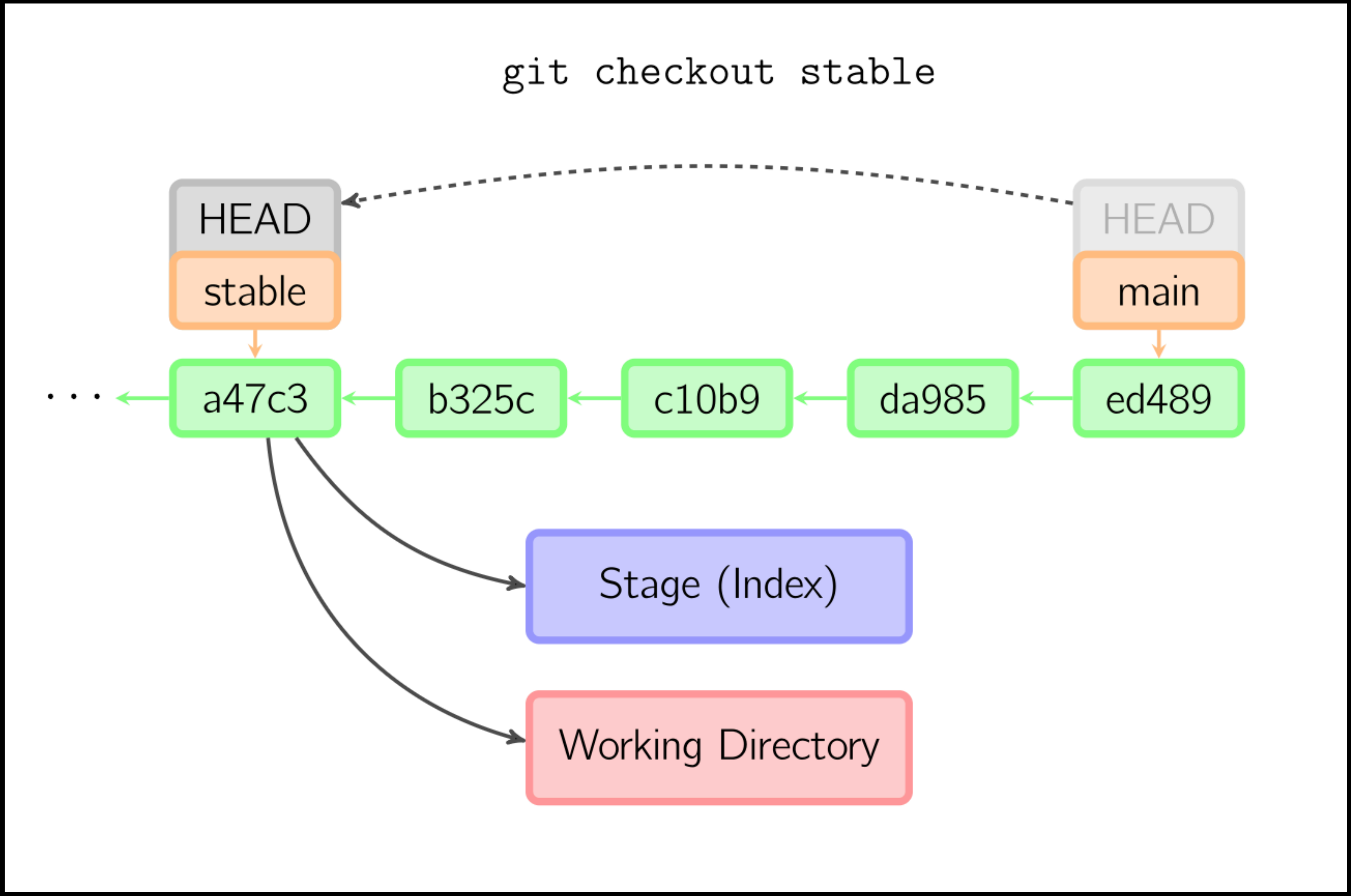


Here we commit while being on the « stable » branch



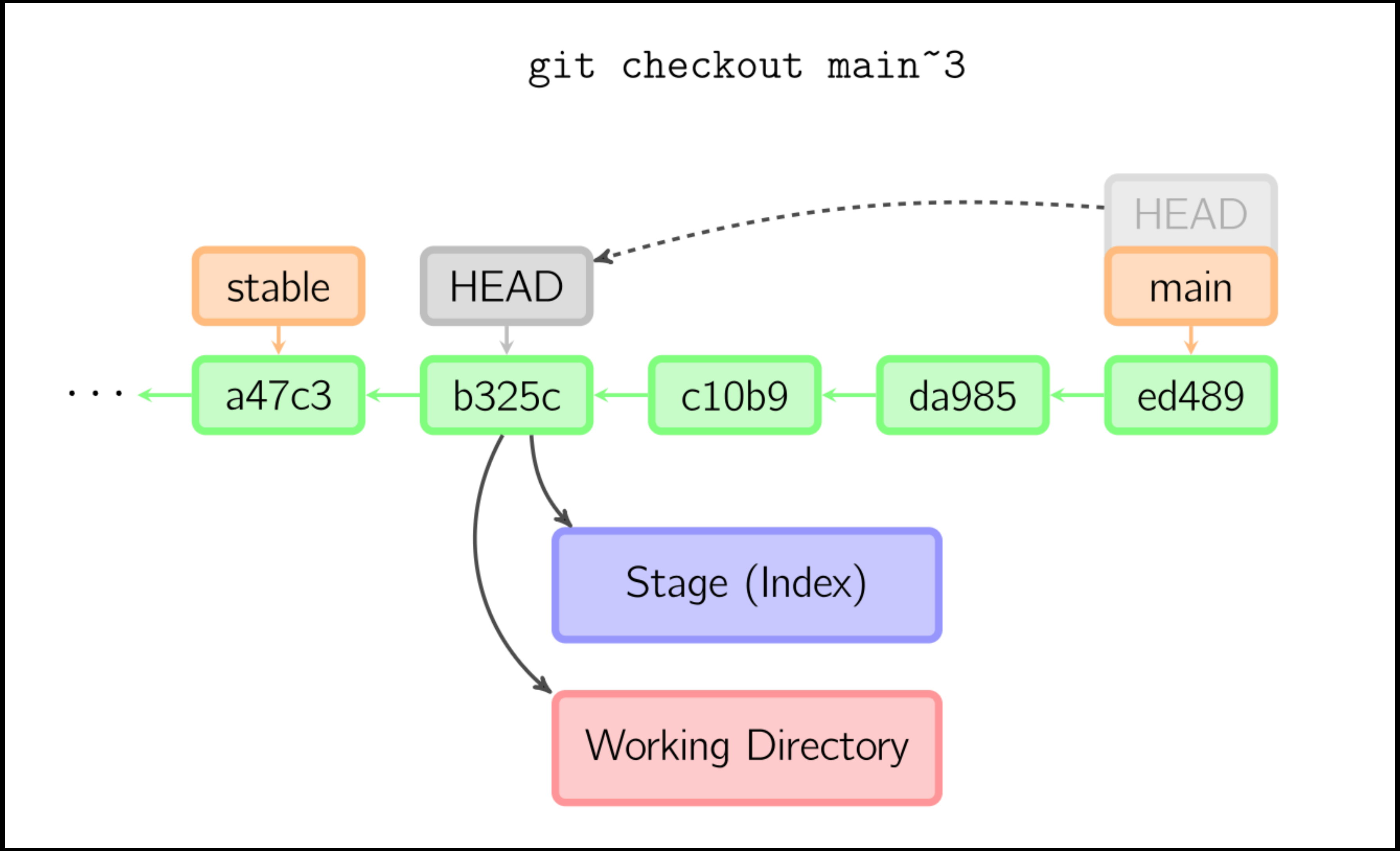
Notice how the history now has a « fork »

You can switch to another branch using git checkout branch-name

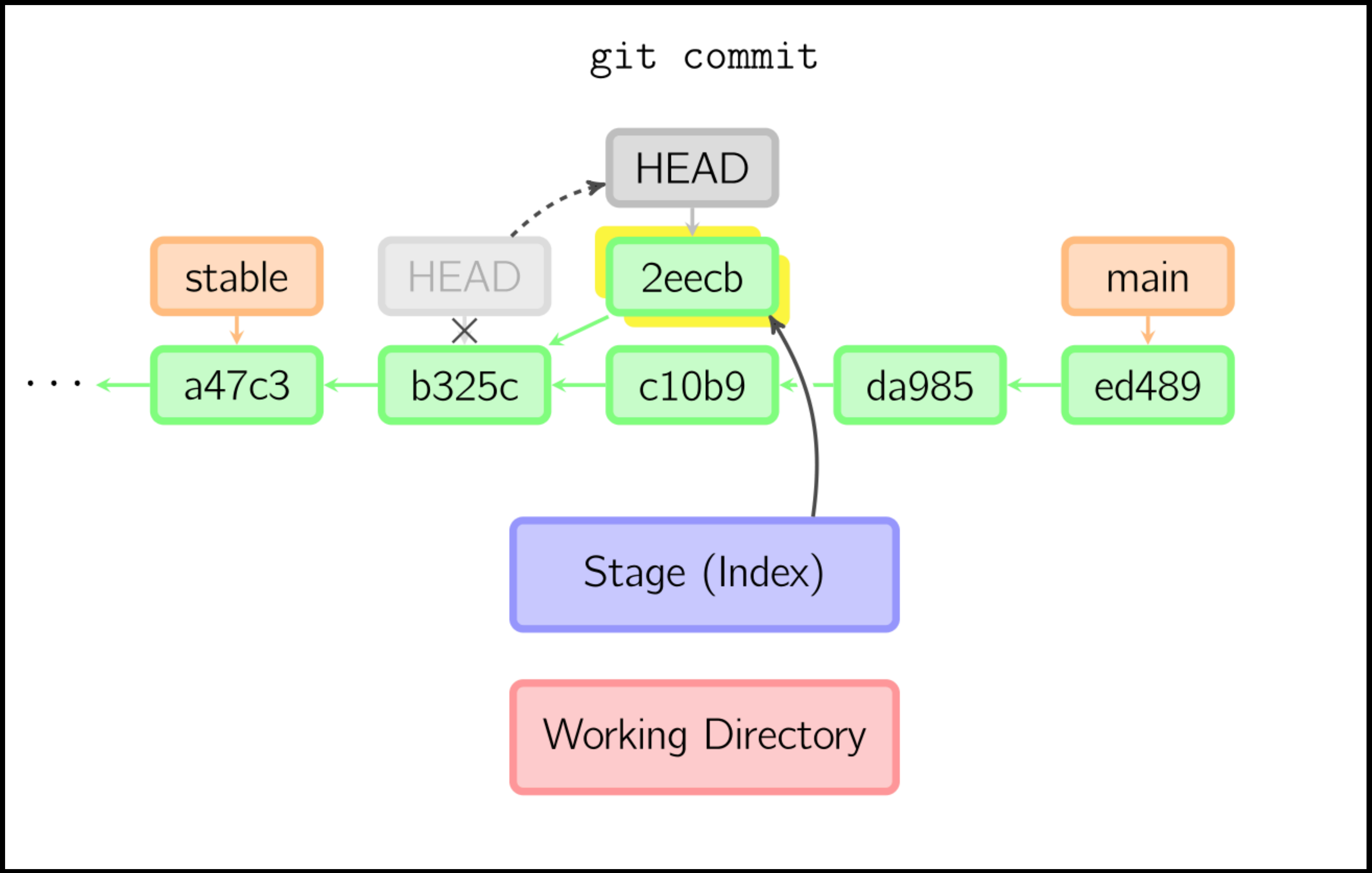


Notice how the history now has a « fork »

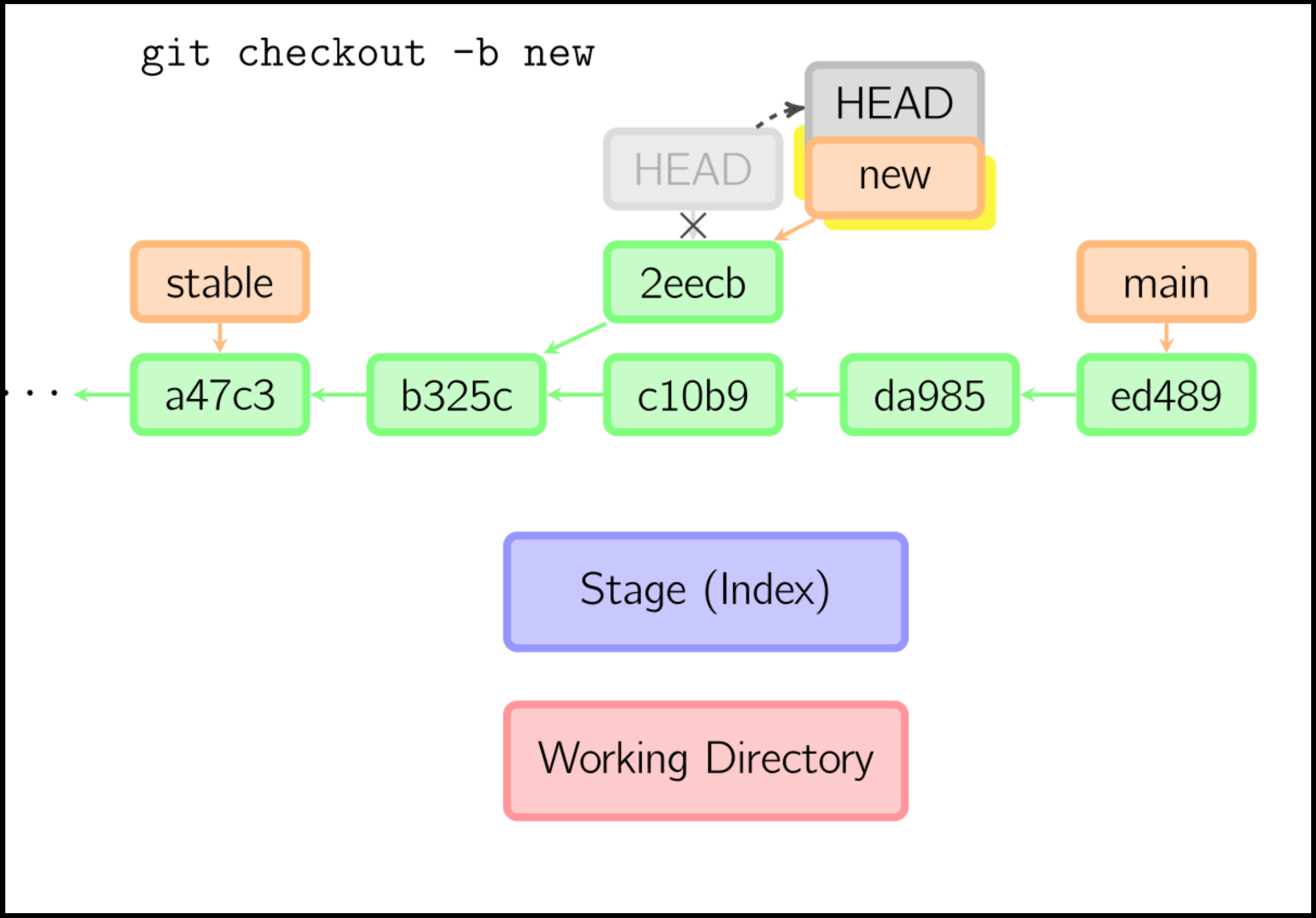
You don't necessarily have to travel to a branch, but can go anywhere in your commit history



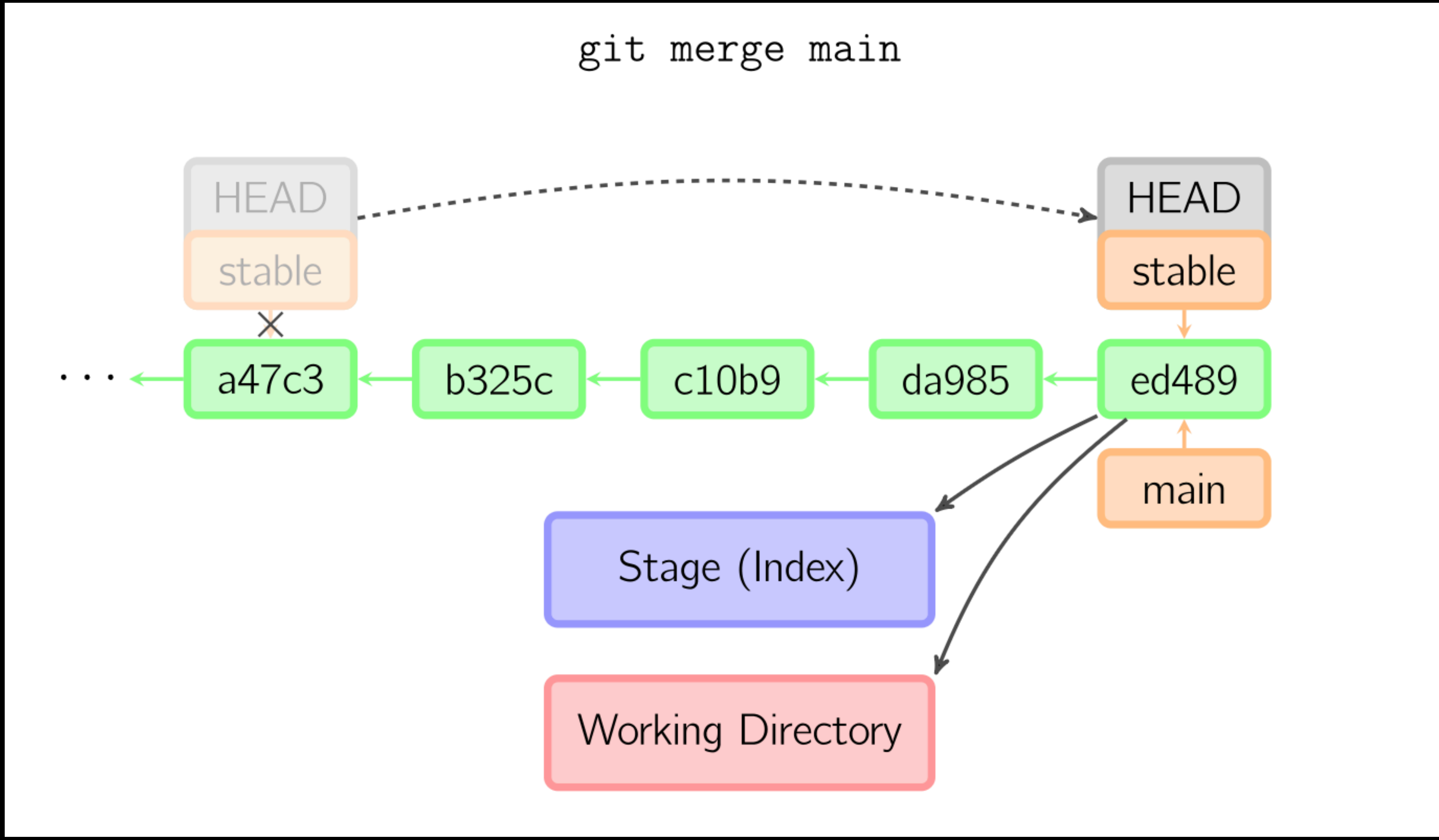
You can even add commits to there



And if you're happy, you can make a new branch from this new commit

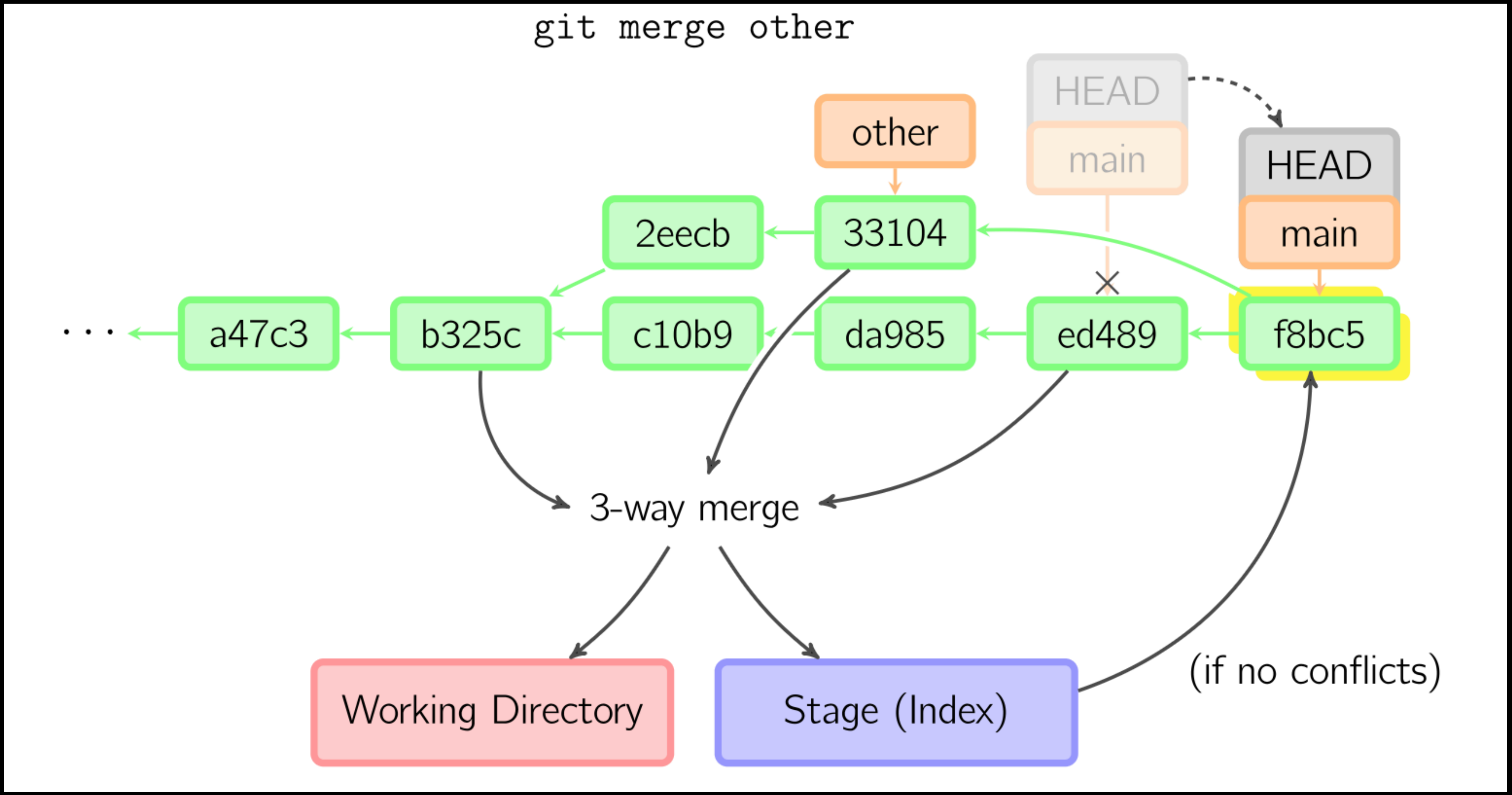


Now you're happy with « main » and want your « stable » branch to catch up with those new developments



The only thing « merge » does here is to move HEAD and 'stable' pointers onto where 'main' points at.

Here the situation is more complex since 'other' has diverged from the history 'main' has

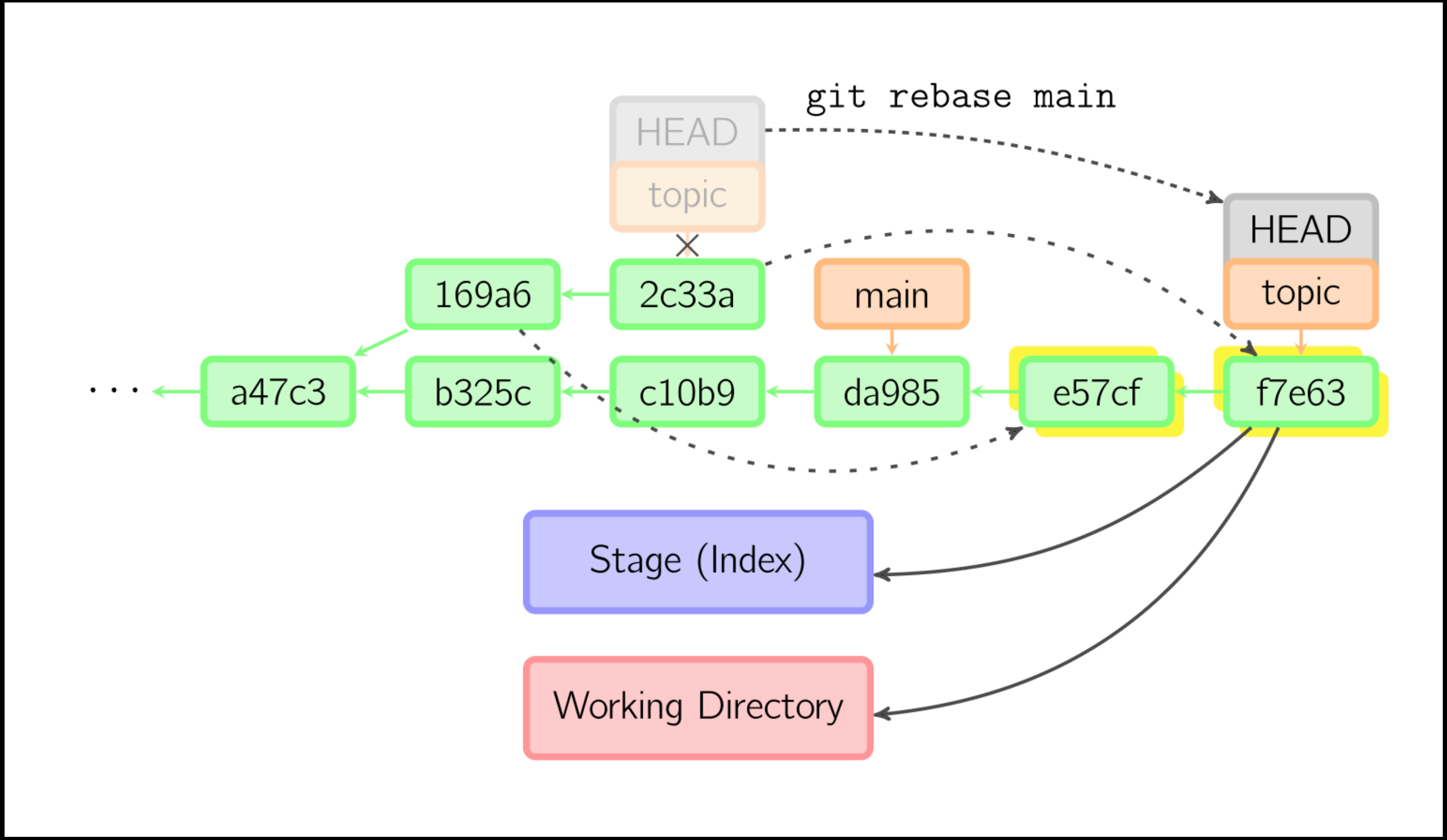


Merge should create a new commit on 'main' from both edits and the common ancestors

If the diverged branches have 'conflicting' edits git will ask you to « resolve » these conflicts

Merge leaves traces in the history, sometimes not worth leaving

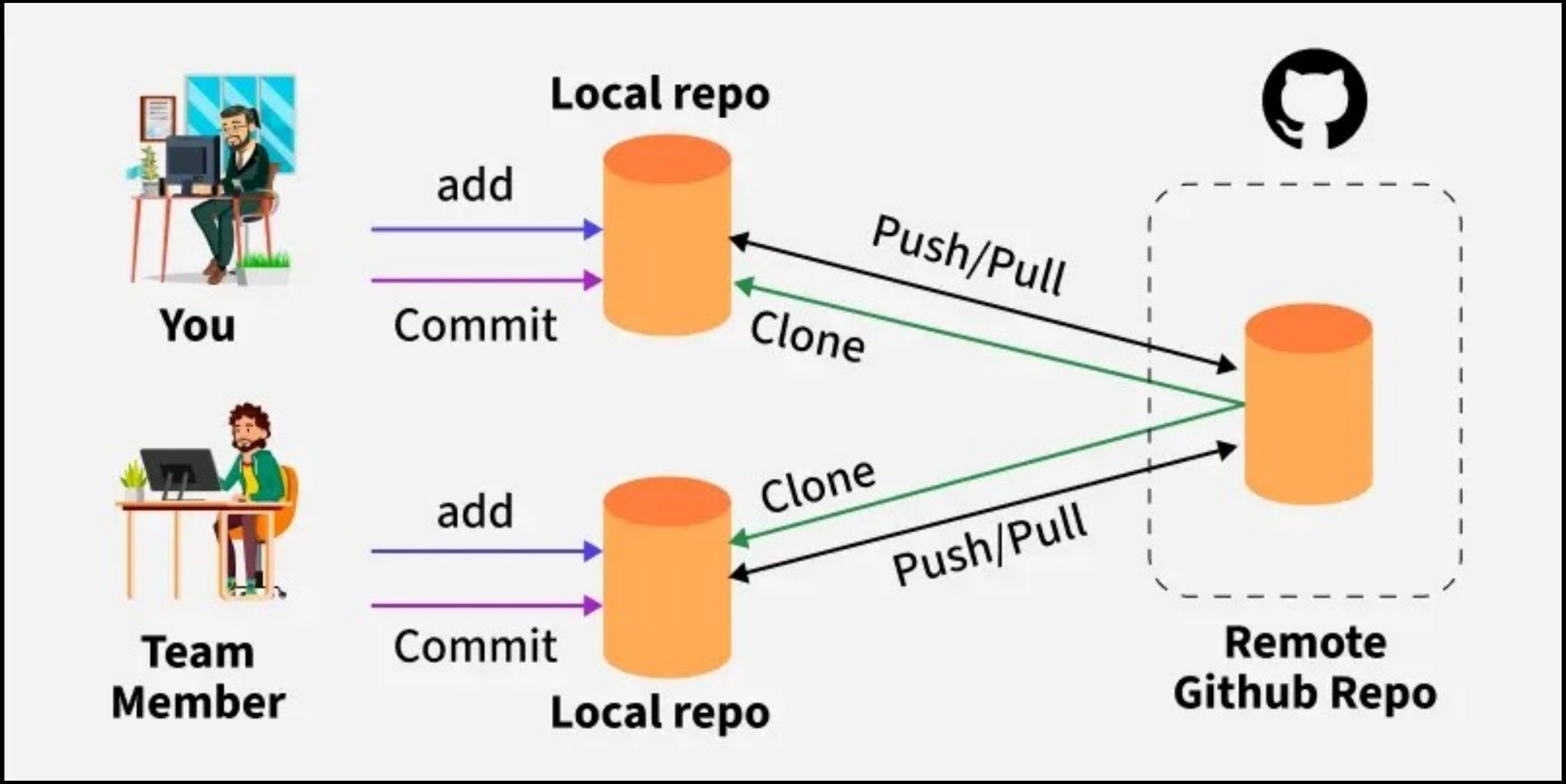
'git rebase' will « rebase » your branch onto the other one



Commits will be played one after the other on top of the destination branch. Conflicts may arise and must be resolved

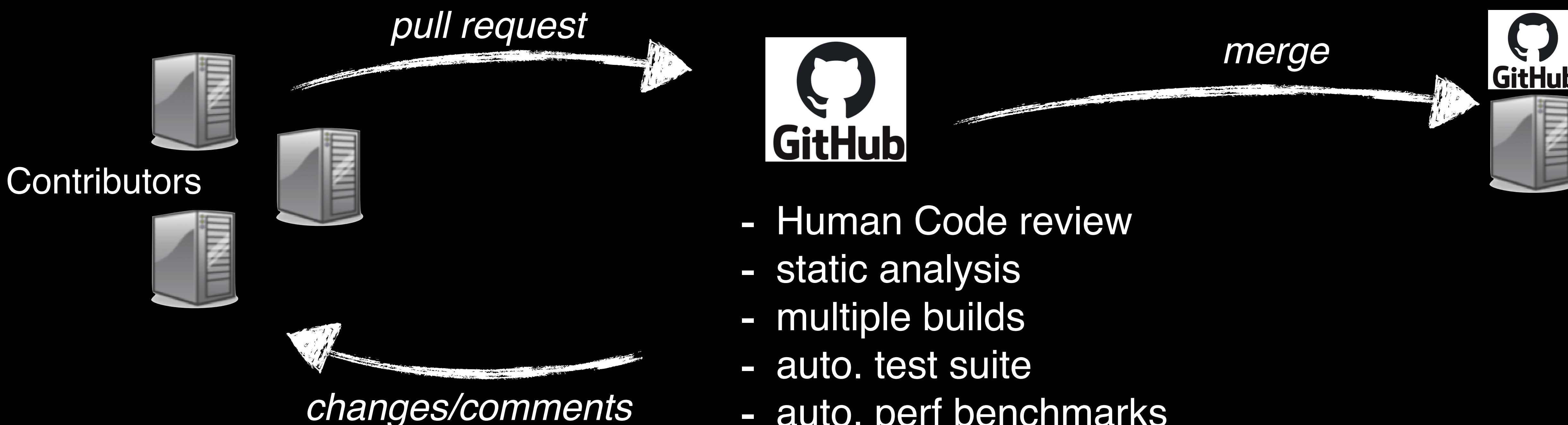
GIT IN A NUTSHELL

- You have your copy of the repository
- Github has a copy
- Your colleague have a version



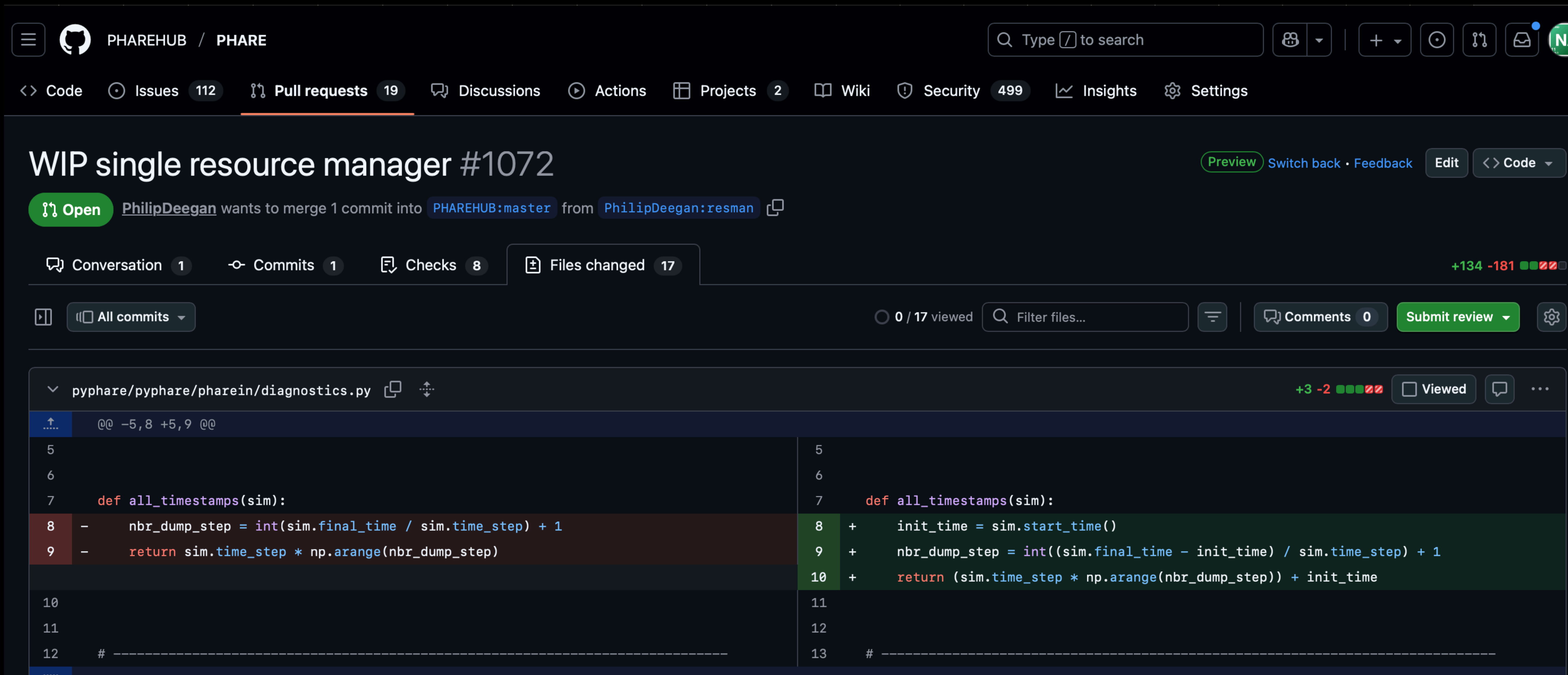
Everyone agrees on the same branches
Everyone can have their own branches

Git in a nutshell



- Human Code review
- static analysis
- multiple builds
- auto. test suite
- auto. perf benchmarks
- code coverage

Git in a Nutshell



See what the new code increment brings, discuss solutions, changes, propose modifications, accepts diff, etc.

Create a Github account

- unit, functional, regression, continuous integration.

HYBRID PARTICLE IN CELL

Hybrid Kinetic Formalism (reminder)

Faraday's law
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$

Ampere's law
$$\mu_0 \, \mathbf{j} = \nabla \times \mathbf{B},$$

Ion Vlasov eq.
$$\frac{\partial f_p}{\partial t} = -\mathbf{v} \cdot \nabla f_p - \frac{\mathbf{E} + \mathbf{v} \times \mathbf{B}}{m_p} \cdot \nabla_{\mathbf{v}} f_p,$$

Ion moments
$$n_i = \sum_p \int f_p(\mathbf{r}, \mathbf{v}) \, d^3 v,$$
$$\mathbf{v}_i = \frac{1}{n_i} \sum_p \int \mathbf{v} \, f_p(\mathbf{r}, \mathbf{v}) \, d^3 v,$$

Quasi-neutrality
$$n_i = n_e = n,$$
$$\mathbf{v}_e = \mathbf{v}_i - \frac{\mathbf{j}}{ne},$$

Generalized Ohm's law
$$\mathbf{E} = -\mathbf{v}_e \times \mathbf{B} - \frac{1}{en} \nabla \cdot \mathbf{P}_e - \frac{m_e}{e} \frac{d\mathbf{v}_e}{dt}.$$

Particle In Cell: a Statistical Lagrangian Approach

Faraday's law
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E},$$

Ampere's law
$$\mu_0 \, \mathbf{j} = \nabla \times \mathbf{B},$$

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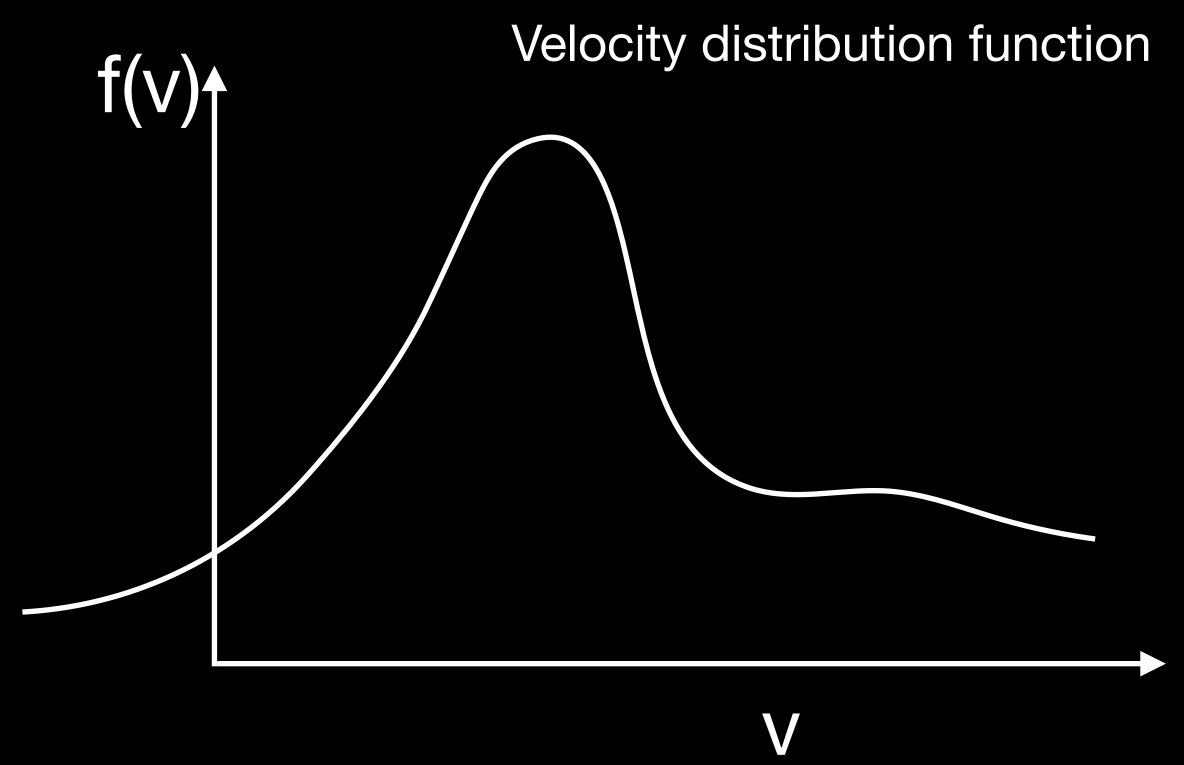
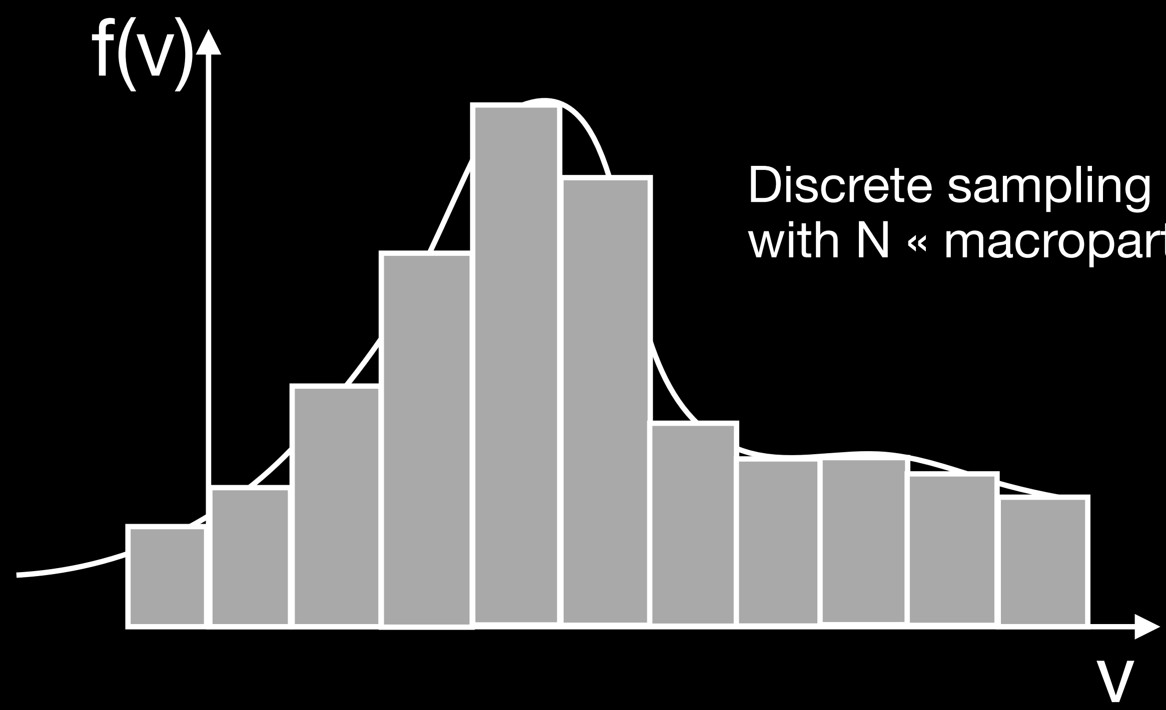
$$\frac{\partial f_p}{\partial t} = -\mathbf{v} \cdot \nabla f_p - \frac{\mathbf{E} + \mathbf{v} \times \mathbf{B}}{m_p} \cdot \nabla_{\mathbf{v}} f_p,$$



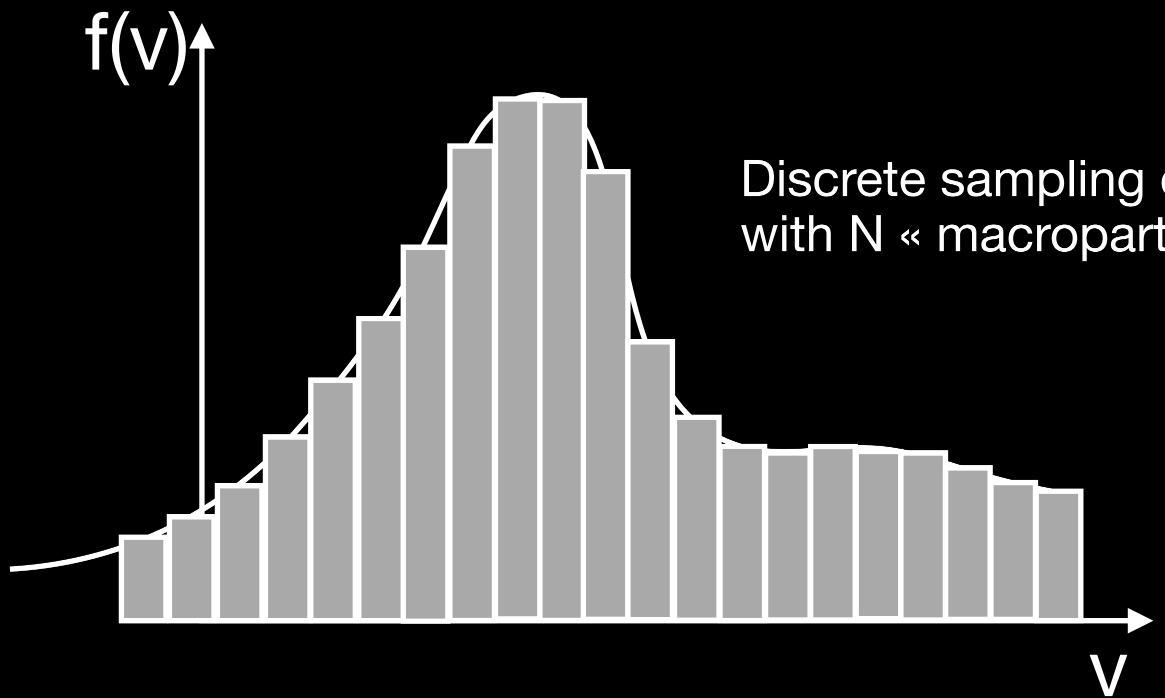
$$\frac{\partial f_p}{\partial t} = -\mathbf{v} \cdot \nabla f_p - \frac{\mathbf{E} + \mathbf{v} \times \mathbf{B}}{m_p} \cdot \nabla_{\mathbf{v}} f_p,$$



Discrete sampling of the distribution with N « macroparticles »

Particle In Cell: a Statistical Lagrangian Approach

$$\frac{\partial f_p}{\partial t} = -\mathbf{v}\cdot\nabla f_p - \frac{\mathbf{E}+\mathbf{v}\times\mathbf{B}}{m_p}\cdot\nabla_{\mathbf{v}} f_p,$$

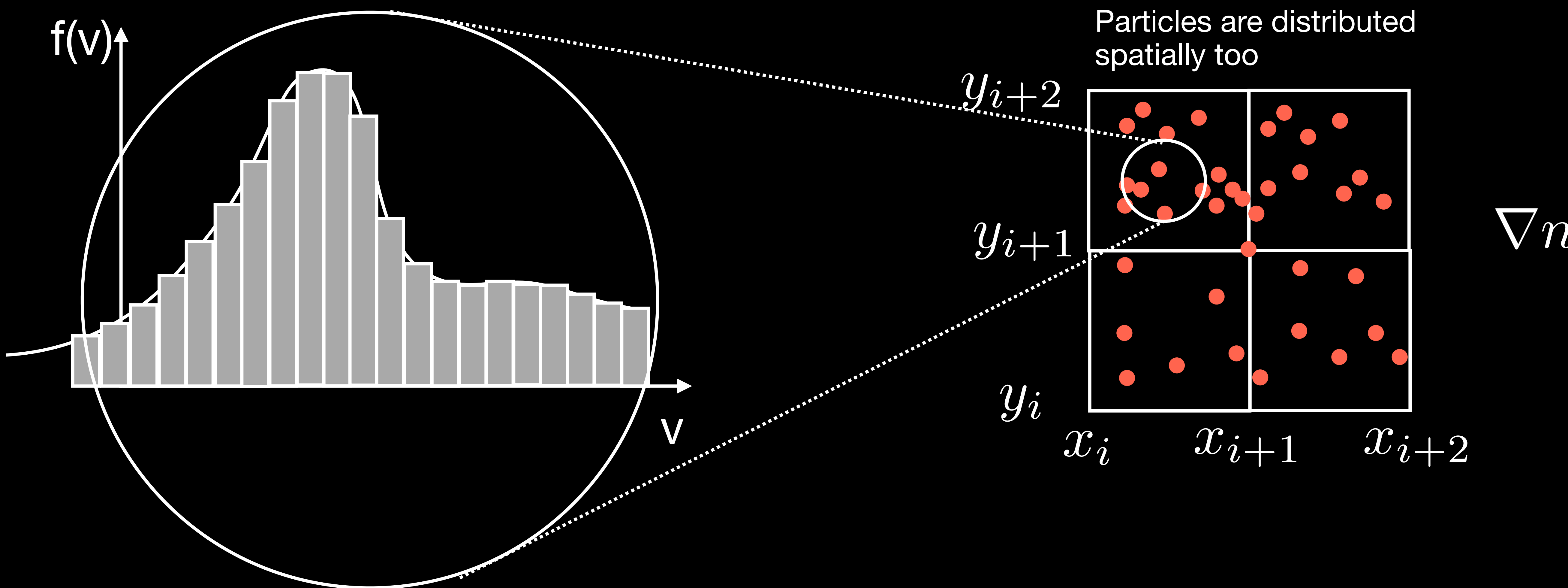


Discrete sampling of the distribution with N « macroparticles »

More particles : better resolution in phase space

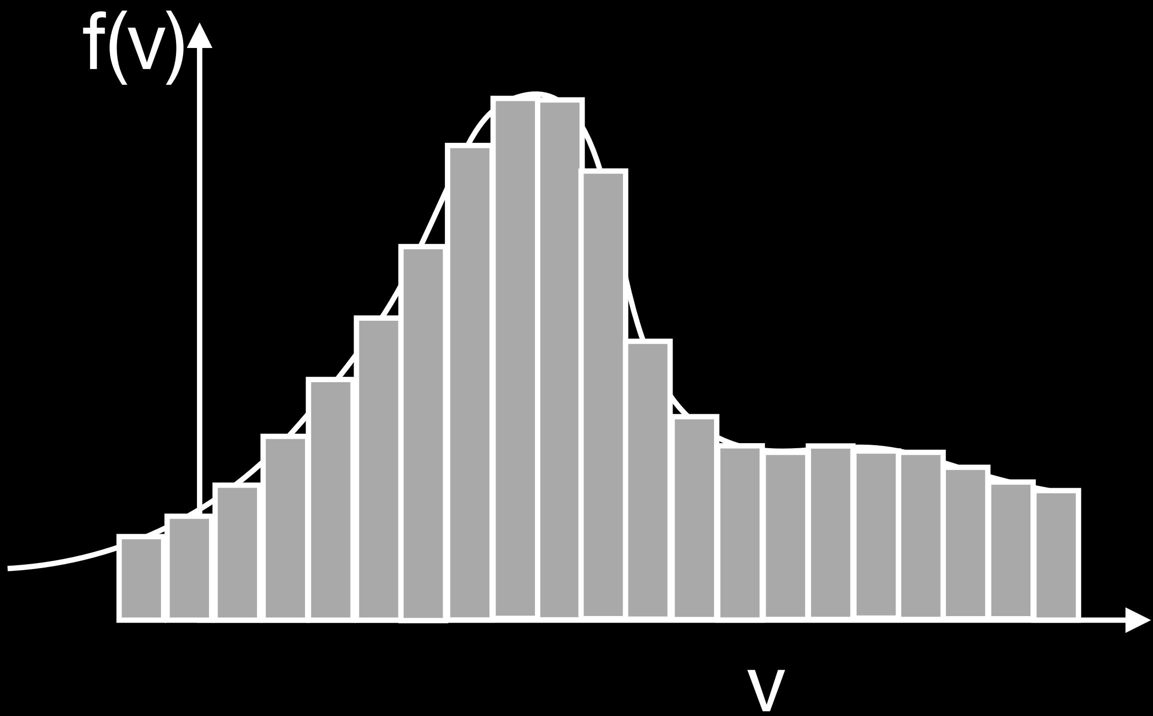
Particle In Cell: a Statistical Lagrangian Approach

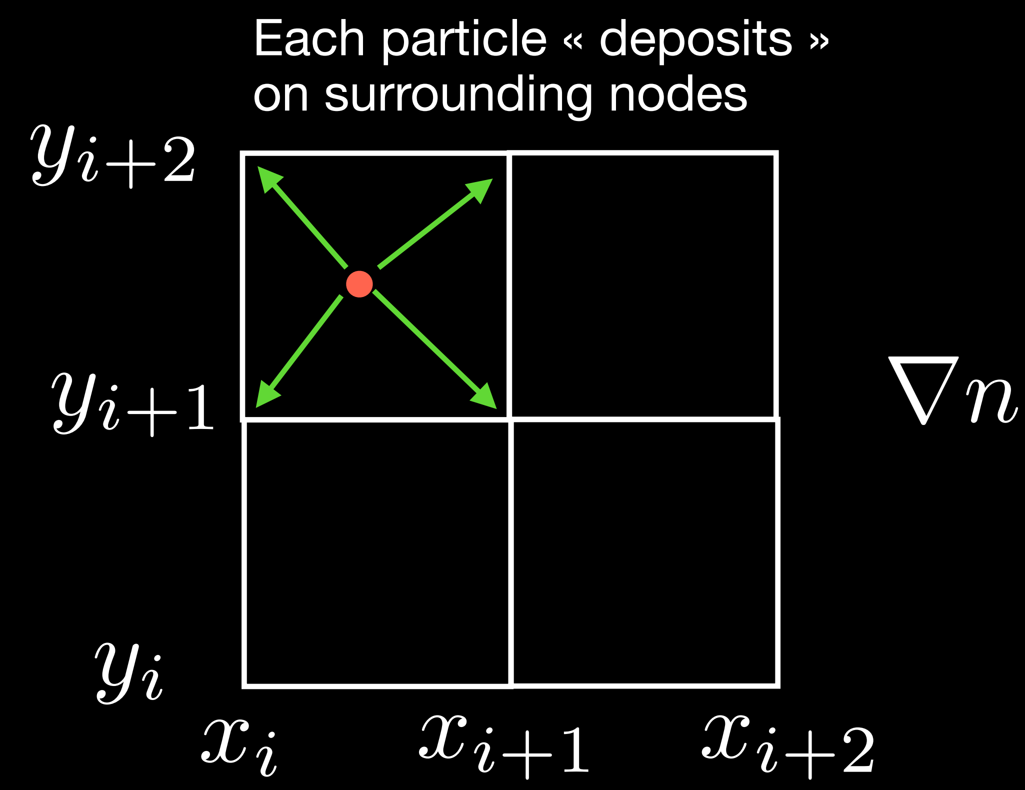
$$\frac{\partial f_p}{\partial t} = -\mathbf{v}\cdot\nabla f_p - \frac{\mathbf{E}+\mathbf{v}\times\mathbf{B}}{m_p}\cdot\nabla_{\mathbf{v}} f_p,$$



$f_p\left(\mathbf{r},\mathbf{v}\right)$ The distribution is discretely sampled in *phase* space

Computing moments of the distribution function on the grid





$$n_i = \sum_p \int f_p(\mathbf{r},\mathbf{v})\, d^3v, \longrightarrow n_{ij} = \sum_p^N S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

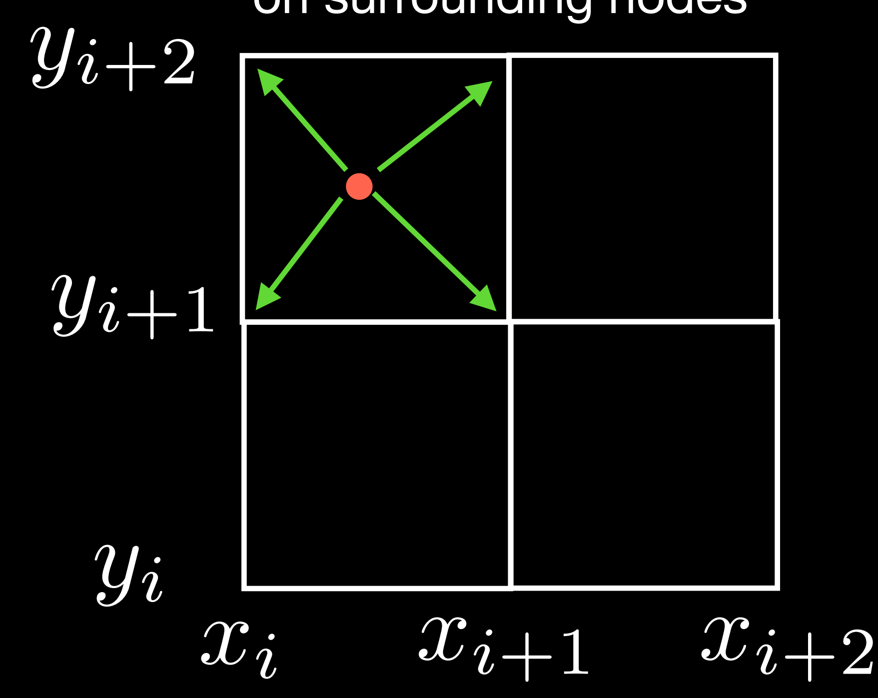
$$\mathbf{v}_i = \frac{1}{n_i} \sum_p \int \mathbf{v}\, f_p(\mathbf{r},\mathbf{v})\, d^3v, \longrightarrow \mathbf{v}_{ij} = \frac{1}{n_{ij}} \sum_p^N \mathbf{v_p} S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

Computing moments of the distribution function on the grid

$$n_{ij} = \sum_{p}^{N} S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

$$\mathbf{v}_{ij} = \frac{1}{n_{ij}} \sum_{p}^{N} \mathbf{v_p} S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

Each particle « deposits » on surrounding nodes

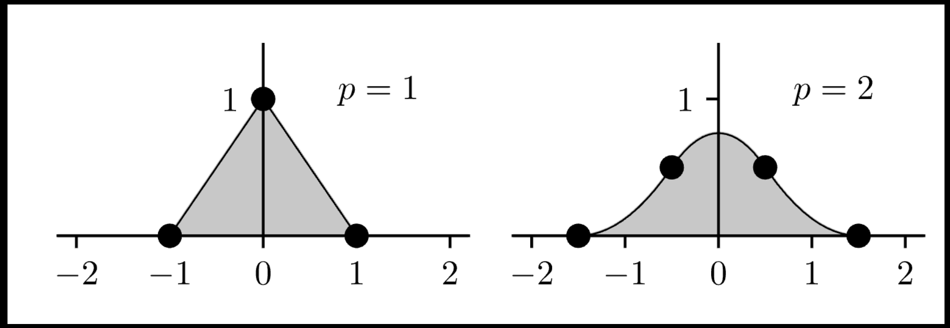


w_p Macroparticle « statistical weight »

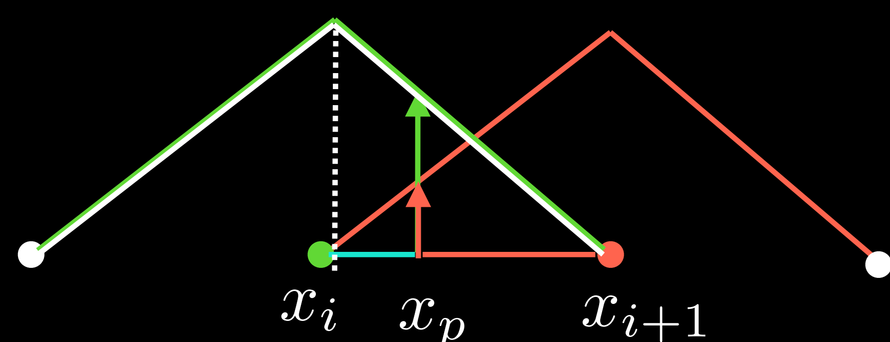
= how much the macro-particle contributes to the local density

Shape function $S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right)$ B-splines

Order 1 is just a linear interpolation



$$n_{i+1} = \frac{(x_p - x_i)}{\Delta x} w_p \qquad n_i = \left(1 - \frac{(x_p - x_i)}{\Delta x}\right) w_p$$

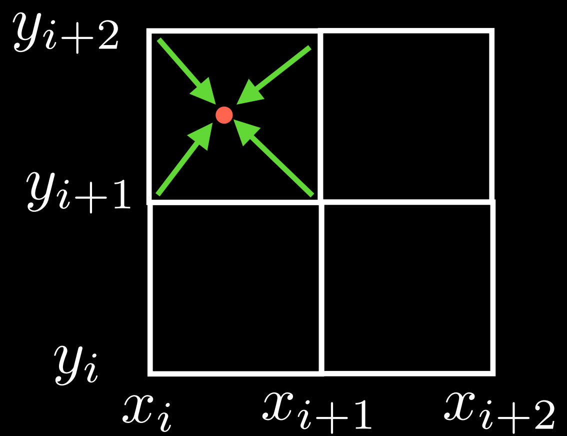


Move particles

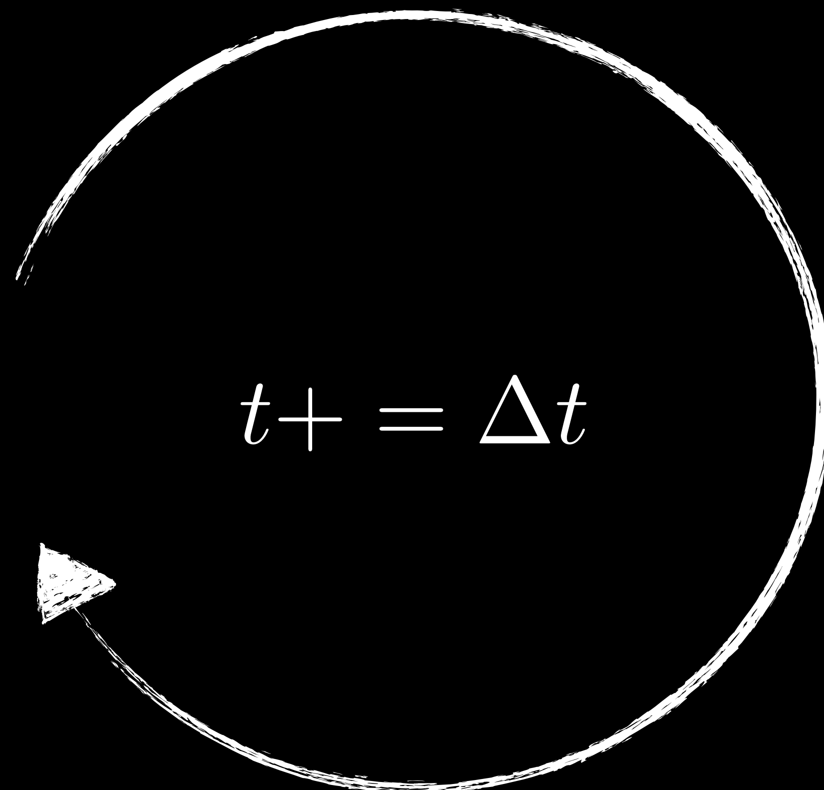
$$m\frac{d\mathbf{v}}{dt} = q\left(\mathbf{E} + \mathbf{v_p} \times \mathbf{B}\right) \qquad \frac{d\mathbf{r_p}}{dt} = \mathbf{v_p}$$

Fields to particles

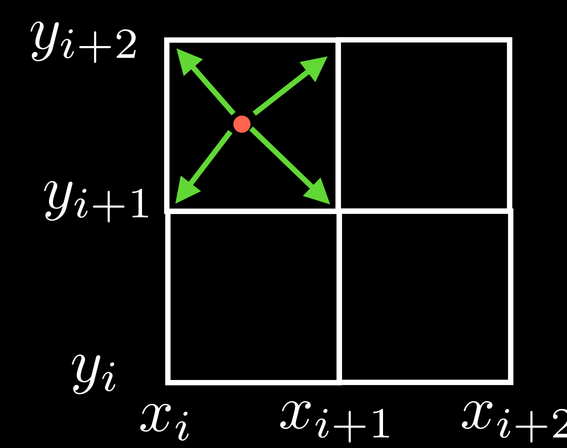
$(\mathbf{E}(\mathbf{r}), \mathbf{B}(\mathbf{r}))$



$$\mathbf{Q}(\mathbf{r}) = \sum_{i=0}^{n-1}\sum_{j=0}^{n-1} Q_{ij}\, S(\mathbf{r_p} - \mathbf{r_{ij}})$$



Accumulate moments



$$n_{ij} = \sum_{p}^{N} S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

$$\mathbf{v}_{ij} = \frac{1}{n_{ij}} \sum_{p}^{N} \mathbf{v_p} S\left(\mathbf{r_p} - \mathbf{r_{ij}}\right) w_p$$

Field equations

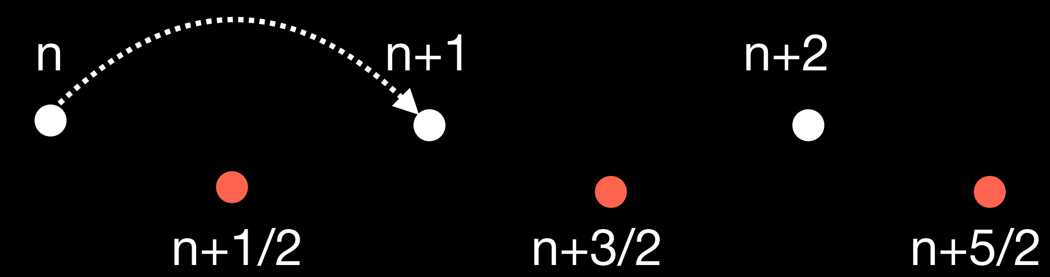
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \qquad \mathbf{v}_e = \mathbf{v}_i - \frac{\mathbf{j}}{ne},$$

$$\mu_0 \mathbf{j} = \nabla \times \mathbf{B}, \qquad \mathbf{E} = -\mathbf{v}_e \times \mathbf{B} - \frac{1}{en}\nabla \cdot \mathbf{P}_e - \frac{m_e}{e}\frac{d\mathbf{v}_e}{dt}.$$

The Boris Pusher

$$\mathbf{r}^{n+1} = \mathbf{r}^n + \boxed{\mathbf{v}^{n+1/2}}\Delta t$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{q\Delta t}{m}\left(\mathbf{E}^{n+\frac{1}{2}} + \boxed{\mathbf{v}^{n+1/2}} \times \mathbf{B}^{n+\frac{1}{2}}\right)$$



The Boris Pusher

Let's assume: $\mathbf{v}^{n+1/2} = \frac{1}{2}\left(\mathbf{v}^n + \mathbf{v}^{n+1}\right)$

Thus $\mathbf{r}^{n+1} = \mathbf{r}^n + \mathbf{v}^{n+1/2}\Delta t$ becomes $\mathbf{r}^{n+1} = \mathbf{r}^n + \frac{1}{2}\left(\mathbf{v}^n + \mathbf{v}^{n+1}\right)\Delta t$

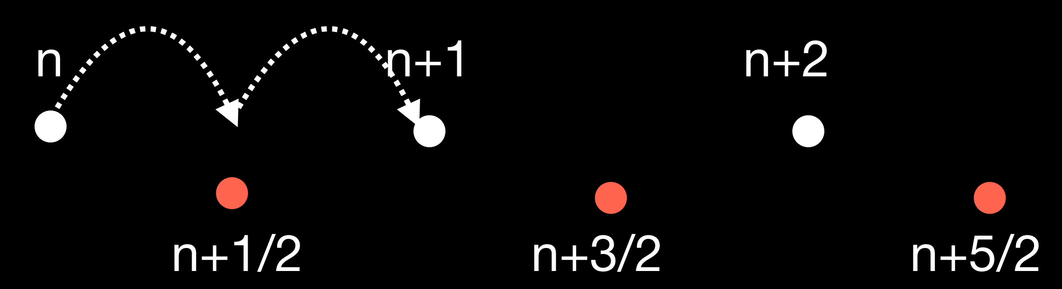
$$\mathbf{r}^{n+1/2} = \mathbf{r}^n + \mathbf{v}^n \frac{\Delta t}{2}$$

$$\mathbf{E}_{ijk}^{n+1/2} \rightarrow \mathbf{E}^{n+1/2}\left(\mathbf{r}^{n+1/2}\right)$$

$$\mathbf{B}_{ijk}^{n+1/2} \rightarrow \mathbf{B}^{n+1/2}\left(\mathbf{r}^{n+1/2}\right)$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{q\Delta t}{m}\left(\mathbf{E}^{n+\frac{1}{2}} + \frac{\mathbf{v}^n + \boxed{\mathbf{v}^{n+1}}}{2} \times \mathbf{B}^{n+\frac{1}{2}}\right)$$

$$\mathbf{r}^{n+1} = \mathbf{r}^{n+1/2} + \mathbf{v}^{n+1}\frac{\Delta t}{2}$$



The Boris Pusher

Let's define: $$\mathbf{v}^n = \mathbf{v}^- - \frac{q\Delta t}{2m}\mathbf{E}^{n+\frac{1}{2}}$$ $$\mathbf{v}^{n+1} = \mathbf{v}^+ + \frac{q\Delta t}{2m}\mathbf{E}^{n+\frac{1}{2}}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{q\Delta t}{m}\left(\mathbf{E}^{n+\frac{1}{2}} + \frac{\mathbf{v}^n + \mathbf{v}^{n+1}}{2} \times \mathbf{B}^{n+\frac{1}{2}}\right)$$

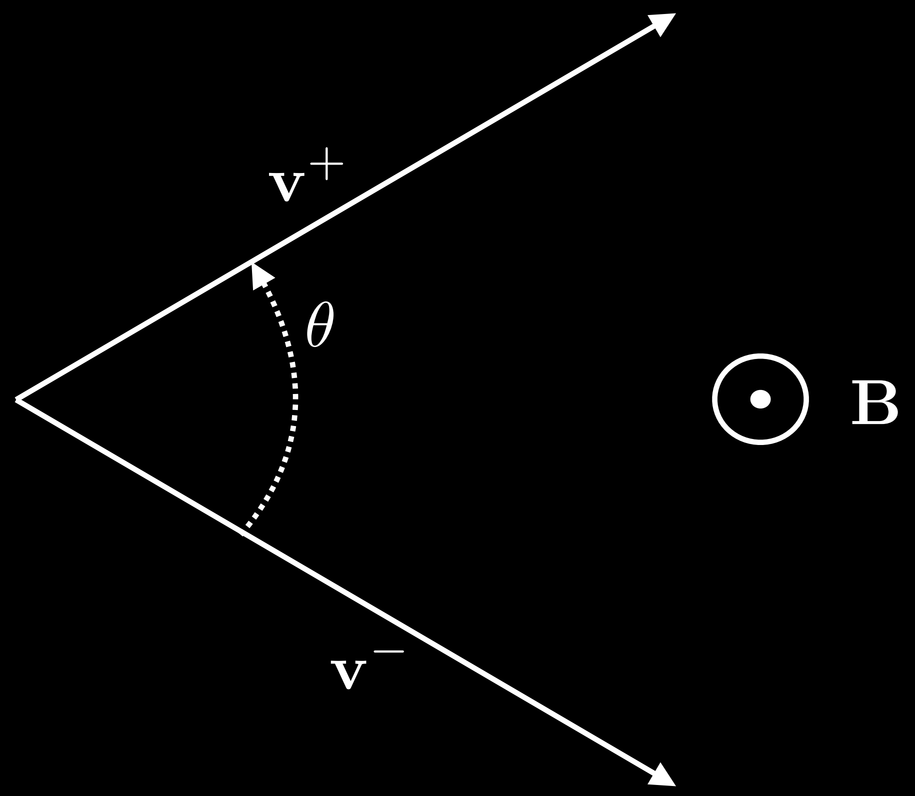
becomes

$$\mathbf{v}^+ - \mathbf{v}^- = \frac{q\Delta t}{2m}\left(\mathbf{v}^+ + \mathbf{v}^-\right) \times \mathbf{B}^{n+1/2}$$

A pure rotation equation conserving energy (no electric work)

Let's focus on the velocity projected in the plane normal to the magnetic field. The parallel component is unchanged in the rotation anyway.

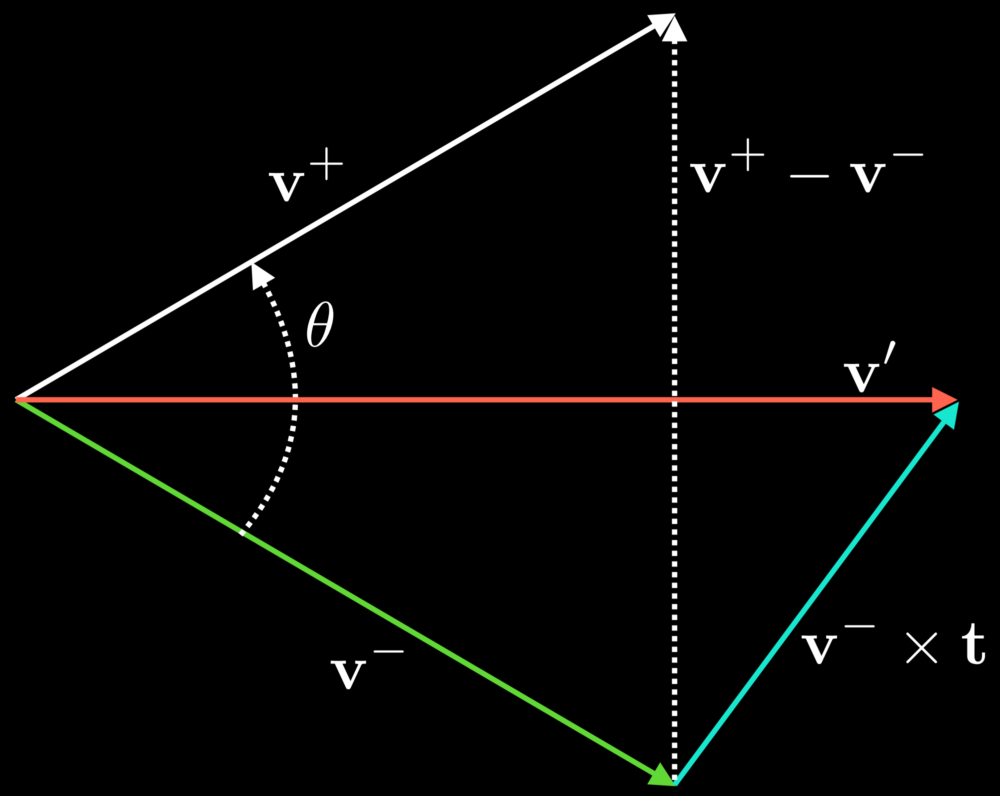
$$\mathbf{v}^+ - \mathbf{v}^- = \frac{q\Delta t}{2m}\left(\mathbf{v}^+ + \mathbf{v}^-\right) \times \mathbf{B}^{n+1/2}$$



$$\mathbf{v}^{+} - \mathbf{v}^{-} = \frac{q\Delta t}{2m}\left(\mathbf{v}^{+} + \mathbf{v}^{-}\right) \times \mathbf{B}^{n+1/2}$$

$$\mathbf{v}' = \mathbf{v}^{-} + \mathbf{v}^{-} \times \mathbf{t}$$

$$\mathbf{t} = \tan\left(\frac{\theta}{2}\right) = \frac{\mathbf{v}^{+} - \mathbf{v}^{-}}{\mathbf{v}^{+} + \mathbf{v}^{-}} = \frac{q\Delta t}{2m} B^{n+1/2}$$



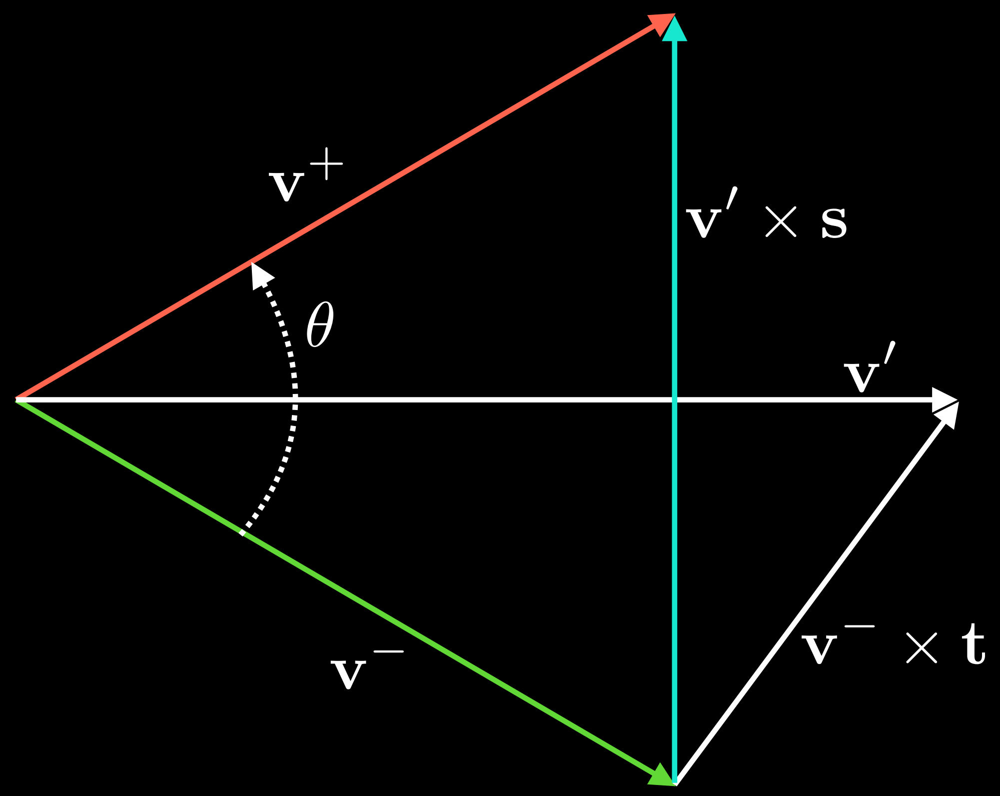
The Boris Pusher

$$\mathbf{v}^+ - \mathbf{v}^- = \frac{q\Delta t}{2m}\left(\mathbf{v}^+ + \mathbf{v}^-\right) \times \mathbf{B}^{n+1/2}$$

$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$$

$$\mathbf{t} = \tan\left(\frac{\theta}{2}\right) = \frac{\mathbf{v}^+ - \mathbf{v}^-}{\mathbf{v}^+ + \mathbf{v}^-} = \frac{q\Delta t}{2m} B^{n+1/2}$$

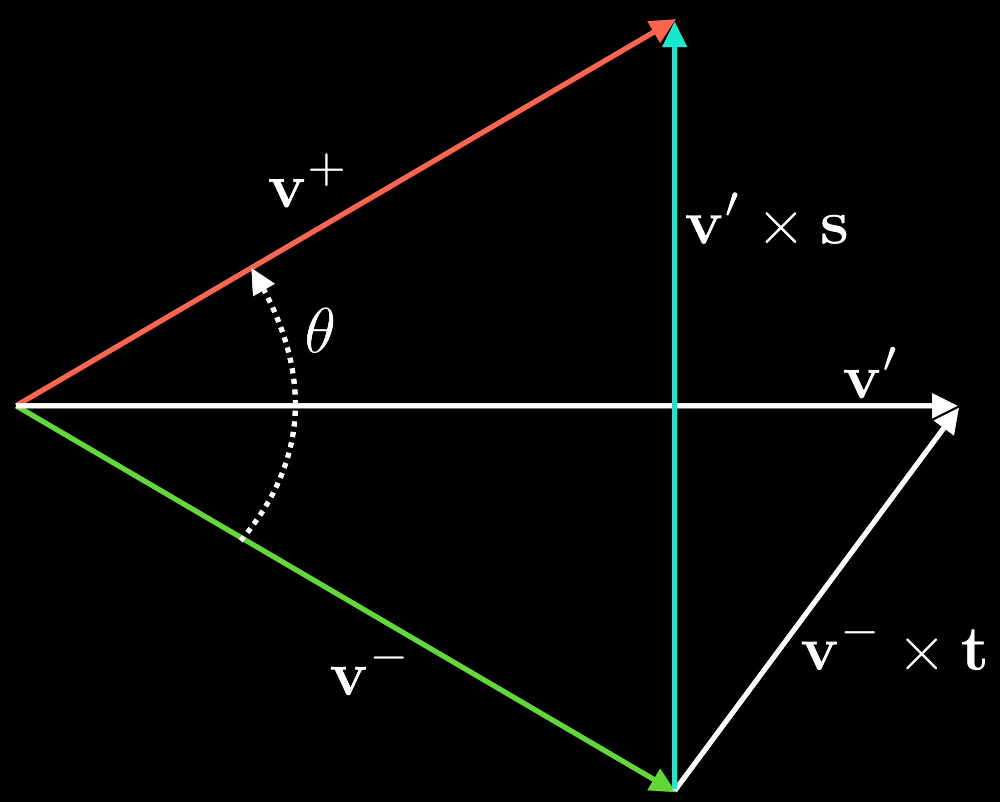
$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$$



$$\mathbf{v}^{+} - \mathbf{v}^{-} = \frac{q\Delta t}{2m}\left(\mathbf{v}^{+} + \mathbf{v}^{-}\right) \times \mathbf{B}^{n+1/2}$$

$$\mathbf{v}' = \mathbf{v}^{-} + \mathbf{v}^{-} \times \mathbf{t}$$

$$\mathbf{v}^{+} = \mathbf{v}^{-} + \mathbf{v}' \times \mathbf{s}$$



$$\cos\left(\theta/2\right) = \frac{v^{-}}{v'} = \frac{v^{+} + v^{-}}{2v^{-}}$$

$$v^{+} + v^{-} = \frac{2(v^{-})^2}{v'^2} v'$$

$$\left(\mathbf{v}^{+} + \mathbf{v}^{-}\right) \times \mathbf{t} = \frac{2(v^{-})^2}{v'^2}\mathbf{v}' \times \mathbf{t}$$

$$\left(\mathbf{v}^{+} - \mathbf{v}^{-}\right) = \frac{2(v^{-})^2}{v'^2}\mathbf{v}' \times \mathbf{t}$$

$$\mathbf{v}' \times \mathbf{s} = \frac{2(v^{-})^2}{v'^2}\mathbf{v}' \times \mathbf{t}$$

$$\mathbf{s} = \frac{2(v^{-})^2}{v'^2}\mathbf{t} \qquad \boxed{\mathbf{s} = \frac{2\mathbf{t}}{1 + t^2}}$$

The Boris Pusher

$$\mathbf{v}^- = \mathbf{v}^n + \frac{q\Delta t}{2m}\mathbf{E}^{n+1/2}$$

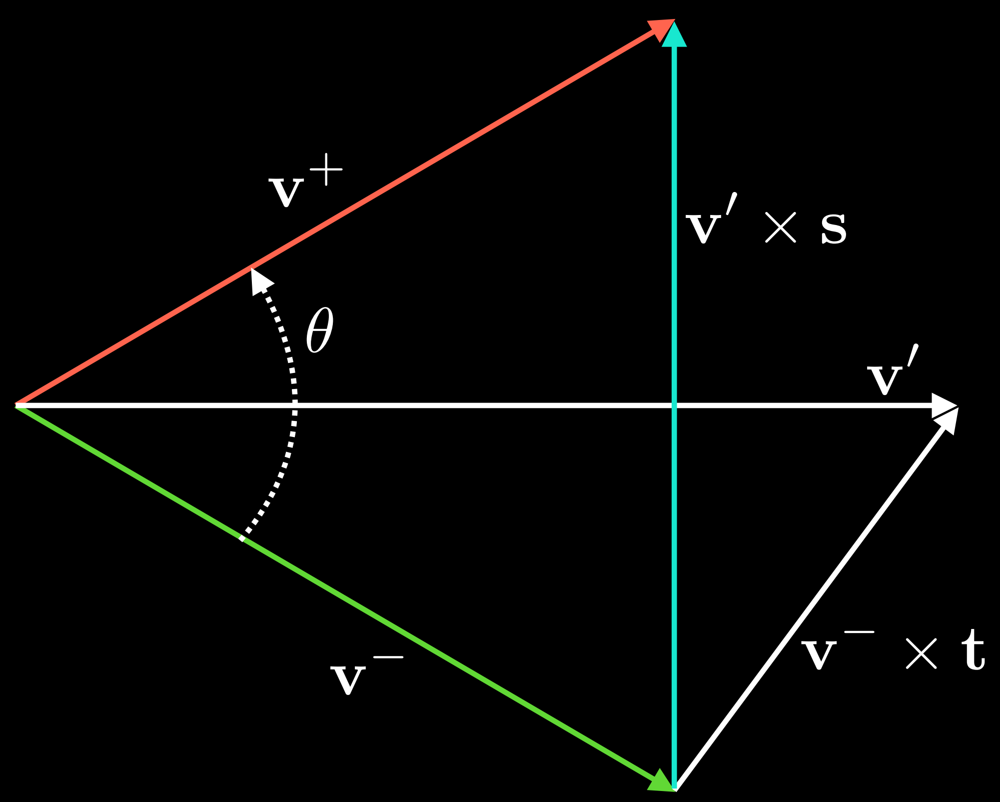
$$\mathbf{t} = \frac{q\Delta t}{2m}\mathbf{B}^{n+1/2}$$

$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$$

$$\mathbf{s} = \frac{2\mathbf{t}}{1+t^2}$$

$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^+ + \frac{q\Delta t}{2m}\mathbf{E}^{n+1/2}$$



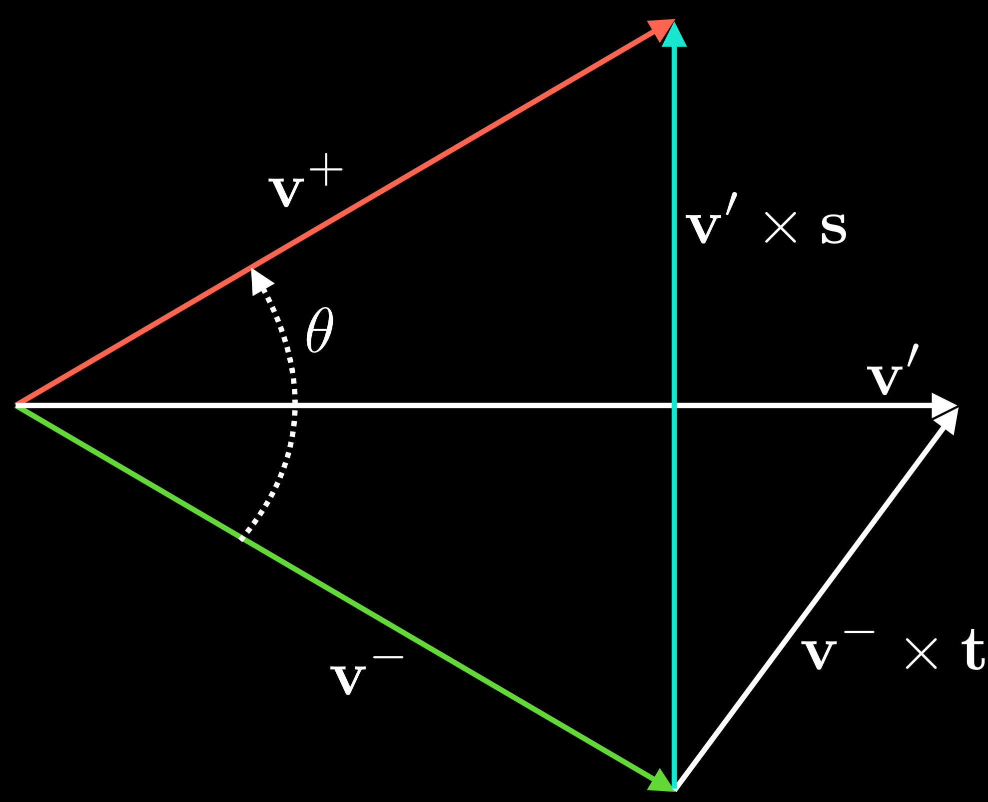
The Boris Pusher

Mid-step position
$$\mathbf{r}^{n+1/2} = \mathbf{r}^n + \mathbf{v}^n \frac{\Delta t}{2}$$

Fields on particle
$$\mathbf{E}^{n+1/2}_{ijk} \to \mathbf{E}^{n+1/2}\left(\mathbf{r}^{n+1/2}\right)$$
$$\mathbf{B}^{n+1/2}_{ijk} \to \mathbf{B}^{n+1/2}\left(\mathbf{r}^{n+1/2}\right)$$

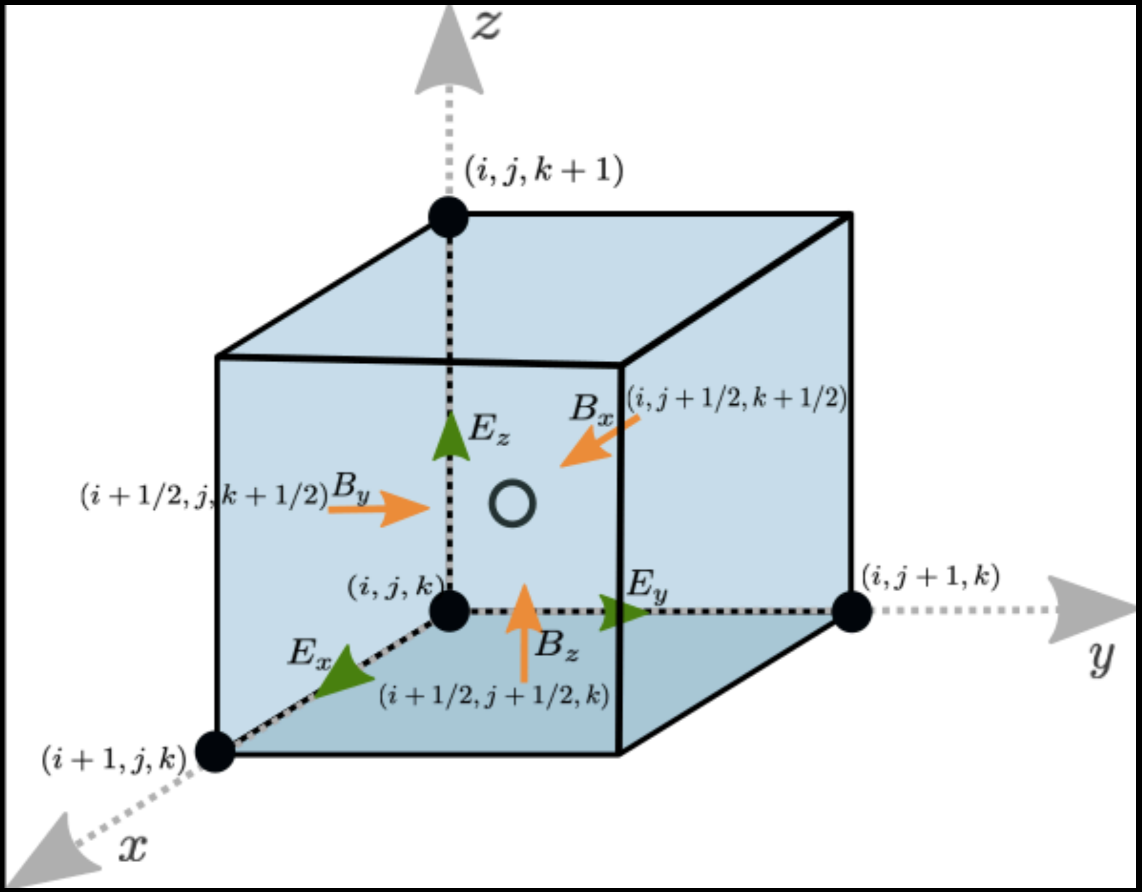
Half electric acceleration
$$\mathbf{v}^- = \mathbf{v}^n + \frac{q\Delta t}{2m}\mathbf{E}^{n+1/2}$$

Magnetic rotation
$$\mathbf{t} = \frac{q\Delta t}{2m}\mathbf{B}^{n+1/2}$$
$$\mathbf{v}' = \mathbf{v}^- + \mathbf{v}^- \times \mathbf{t}$$
$$\mathbf{s} = \frac{2\mathbf{t}}{1+t^2}$$
$$\mathbf{v}^+ = \mathbf{v}^- + \mathbf{v}' \times \mathbf{s}$$



Half electric acceleration
$$\mathbf{v}^{n+1} = \mathbf{v}^+ + \frac{q\Delta t}{2m}\mathbf{E}^{n+1/2}$$

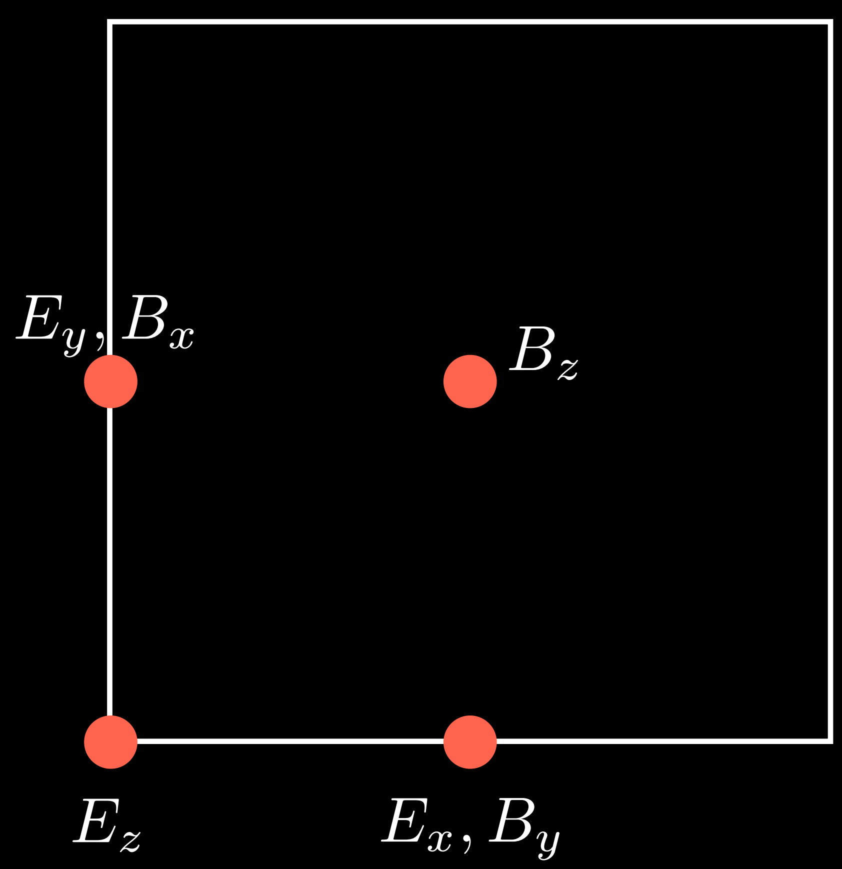
Final position
$$\mathbf{r}^{n+1} = \mathbf{r}^{n+1/2} + \mathbf{v}^{n+1}\frac{\Delta t}{2}$$

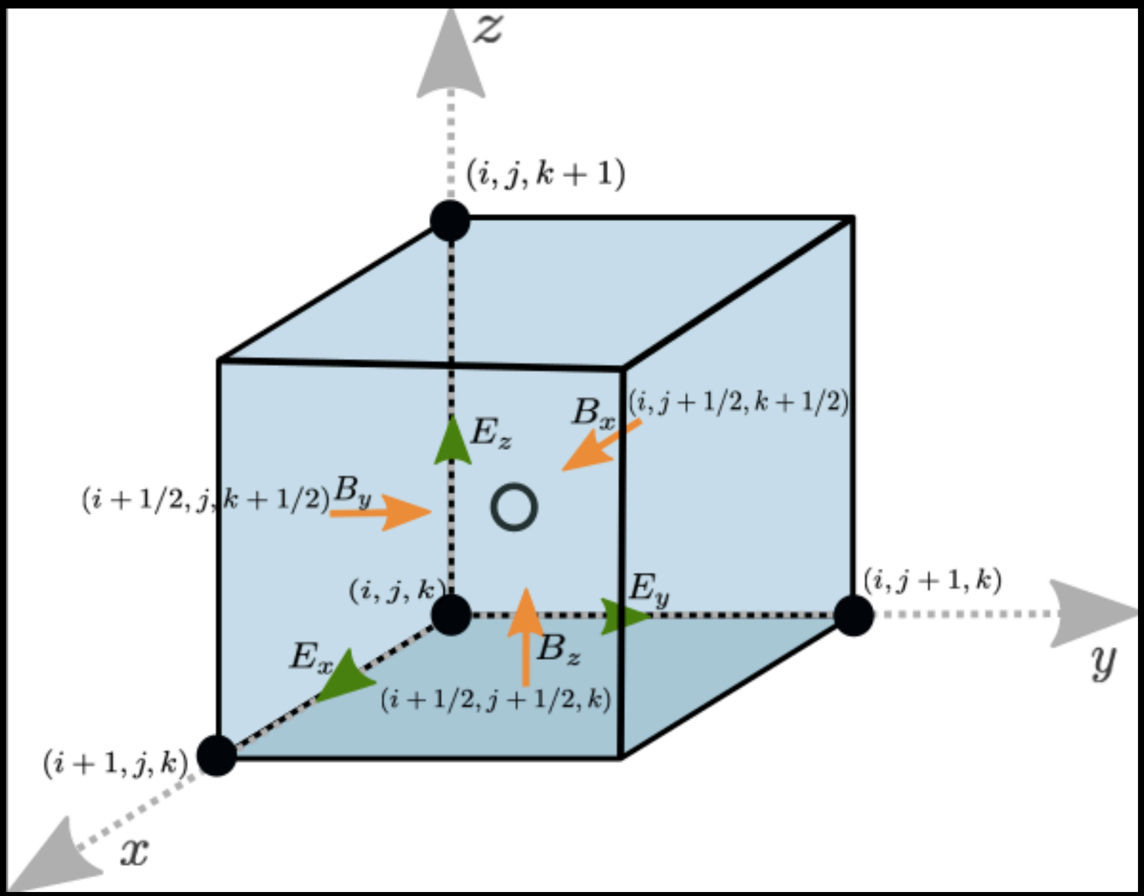


Magnetic components on faces
Electric components on edges

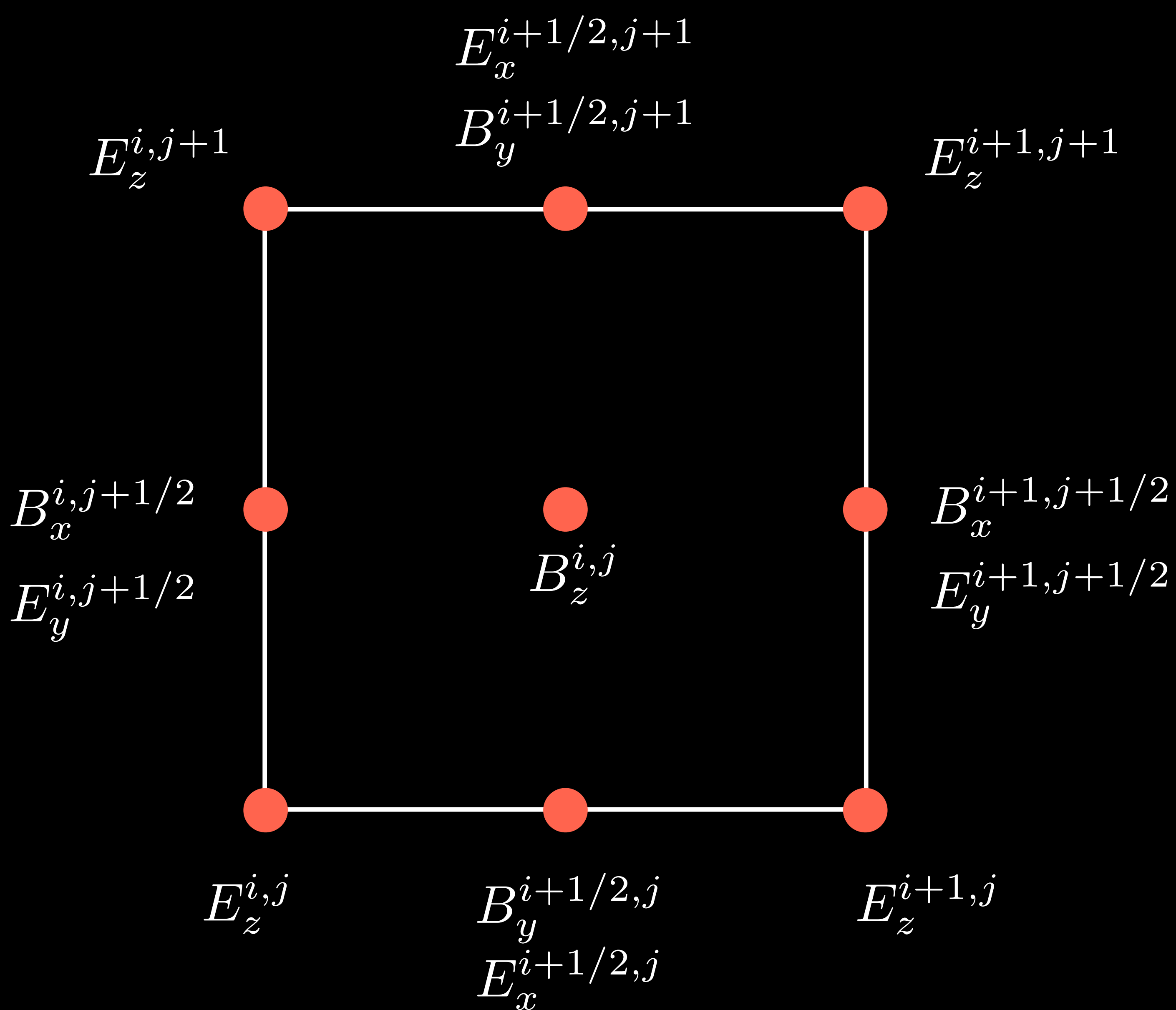
The Yee Mesh Layout

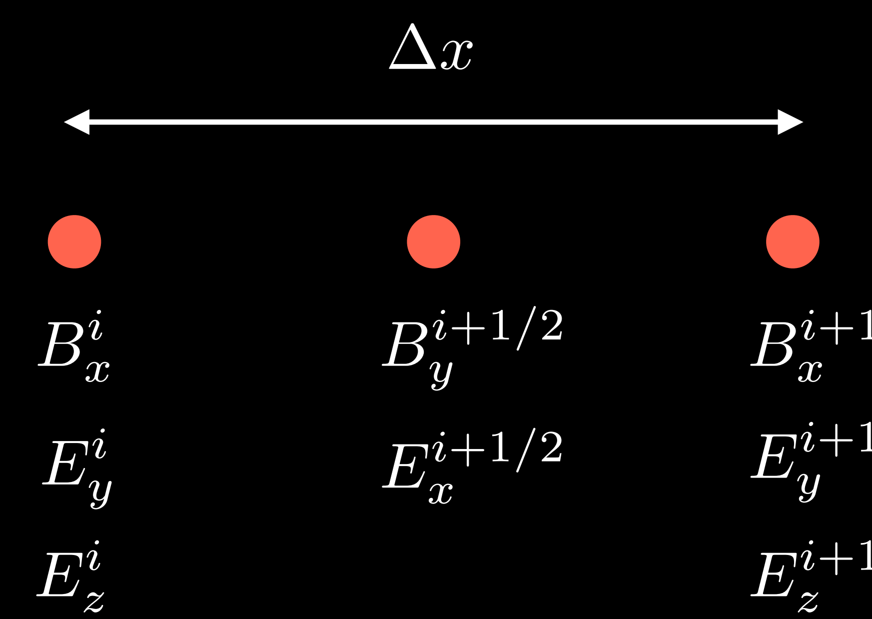
2D yee cell





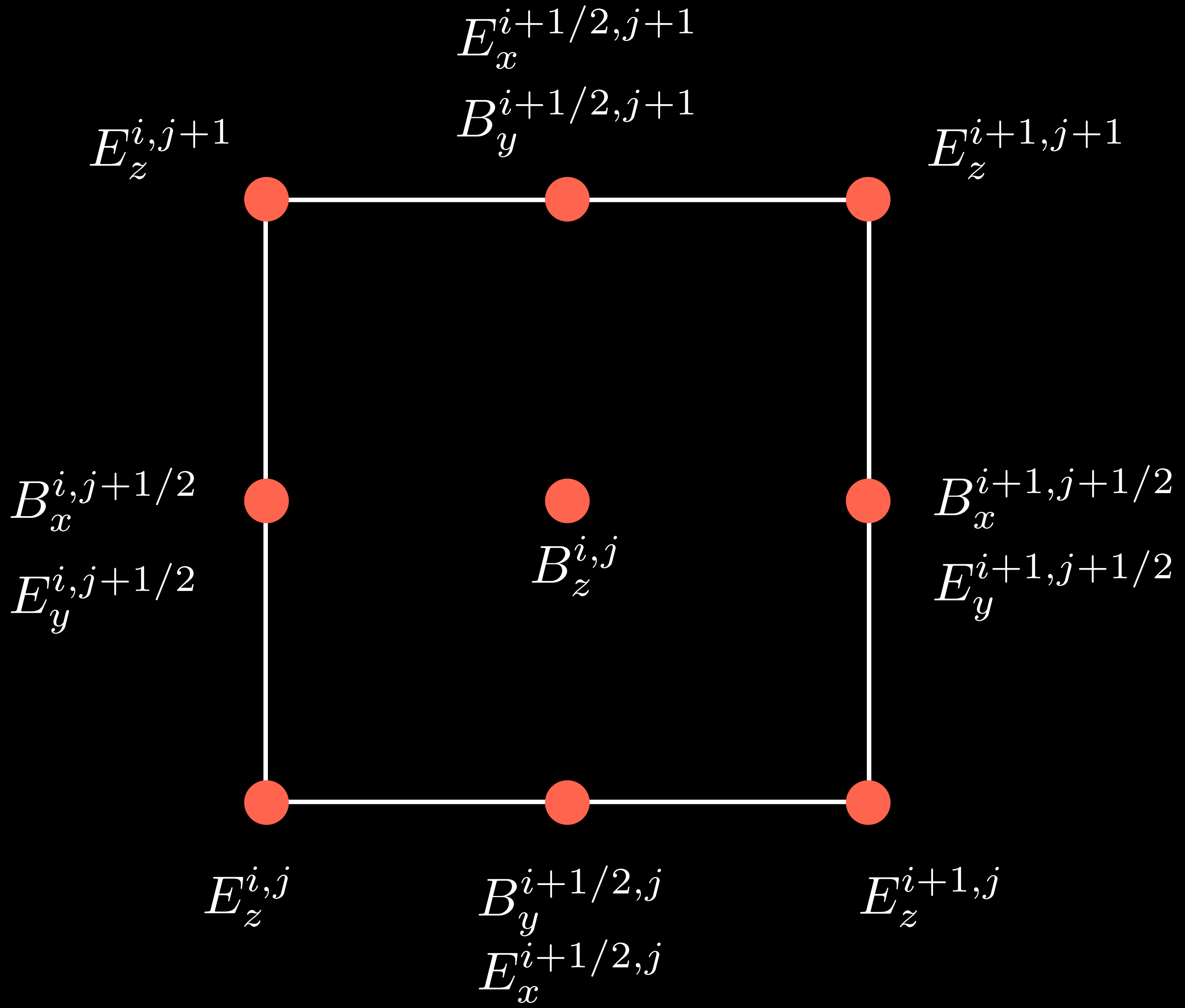
The 2D and 1D Yee Mesh Layout





Why doing something « so complicated? »

Why so (apparently) complicated?



curl

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

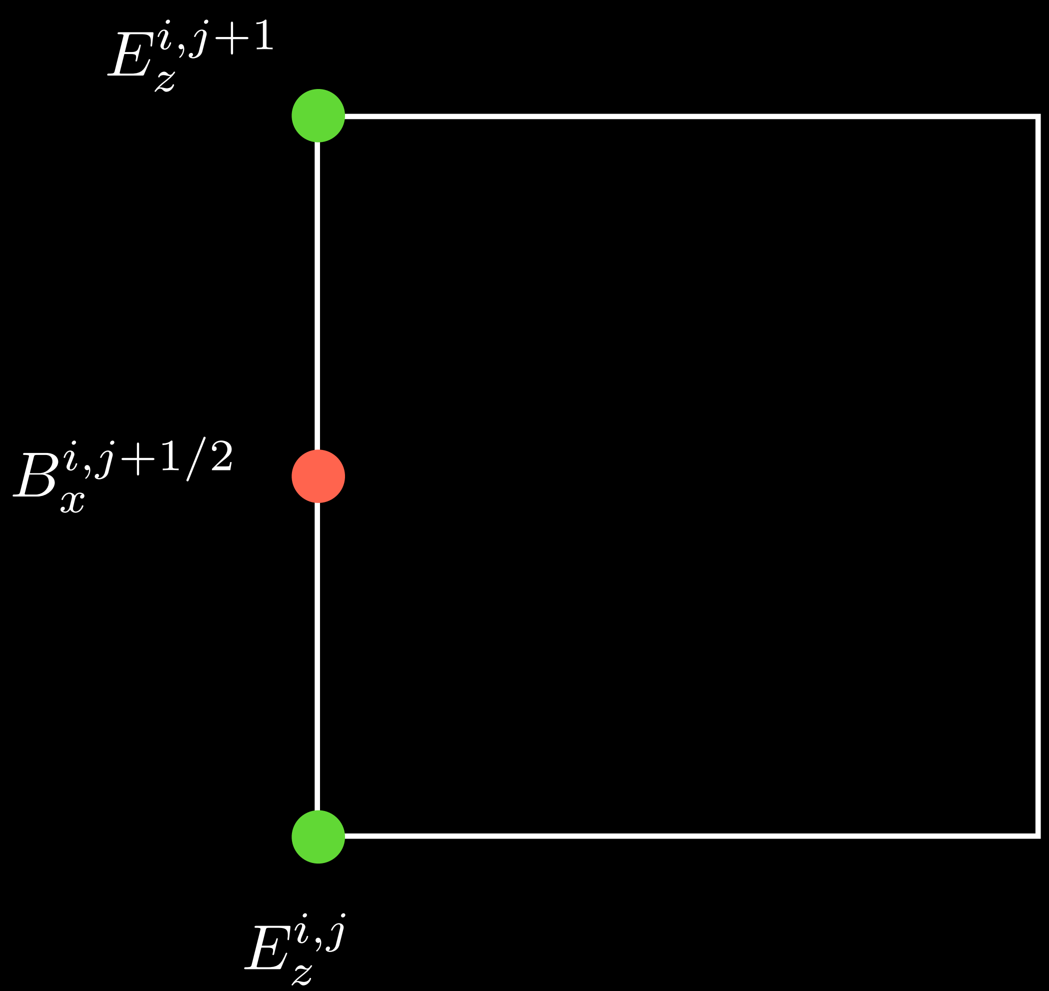
First order derivative

$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y}$$

$$\frac{\partial B_y}{\partial t} = \frac{\partial E_z}{\partial x}$$

$$\frac{\partial B_z}{\partial t} = \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}$$

Why so (apparently) complicated?



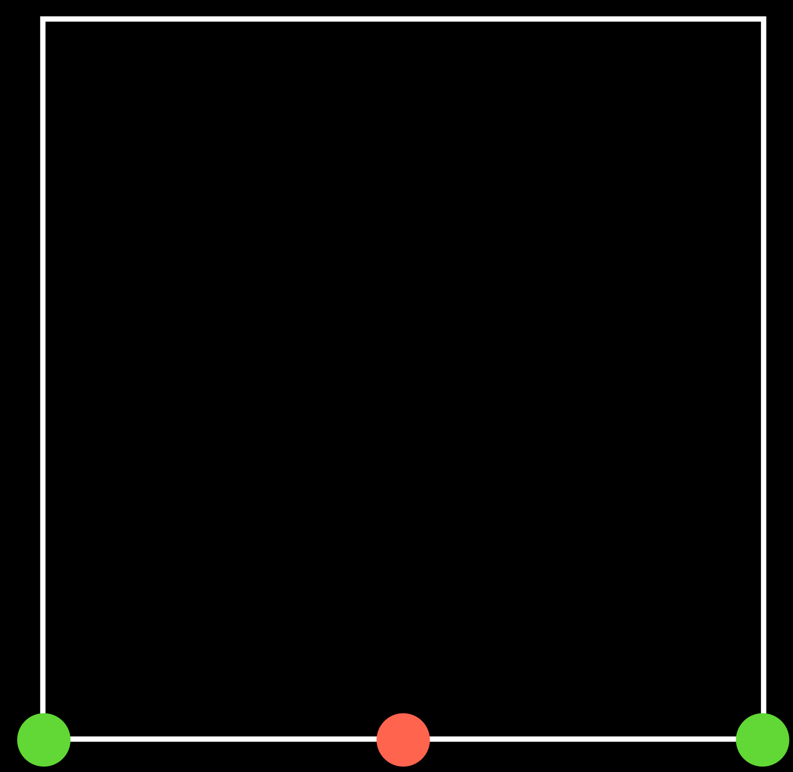
$$\frac{\partial \mathbf{B}}{\partial t} = -\underset{\text{First order derivative}}{\nabla} \overset{\text{curl}}{\times} \mathbf{E}$$

$$\boxed{\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y}}$$

$$\frac{\partial B_y}{\partial t} = \frac{\partial E_z}{\partial x}$$

$$\frac{\partial B_z}{\partial t} = \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}$$

Why so (apparently) complicated?



curl

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First order derivative

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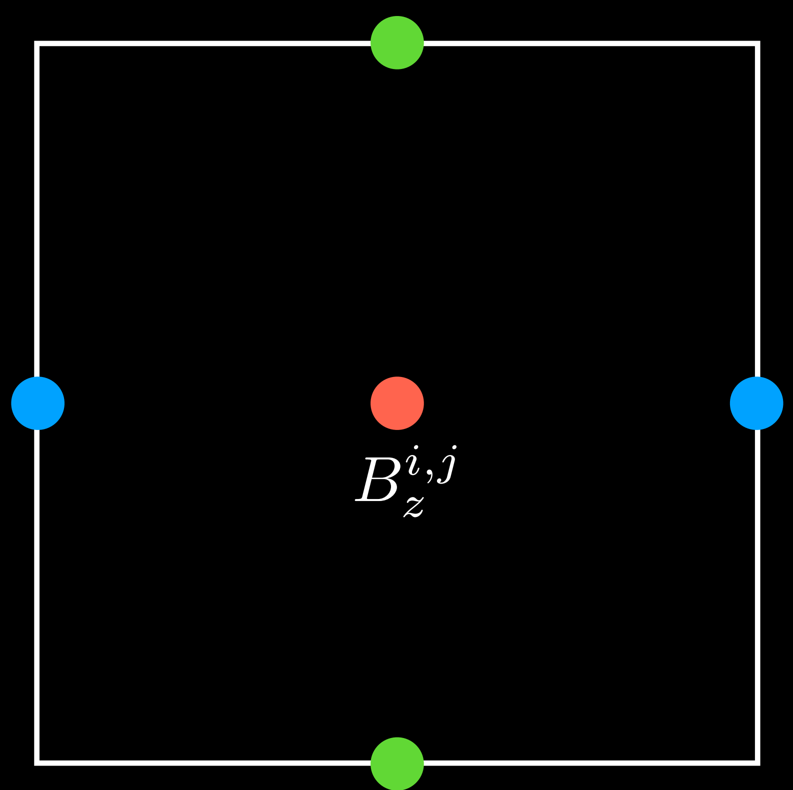

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First order derivative

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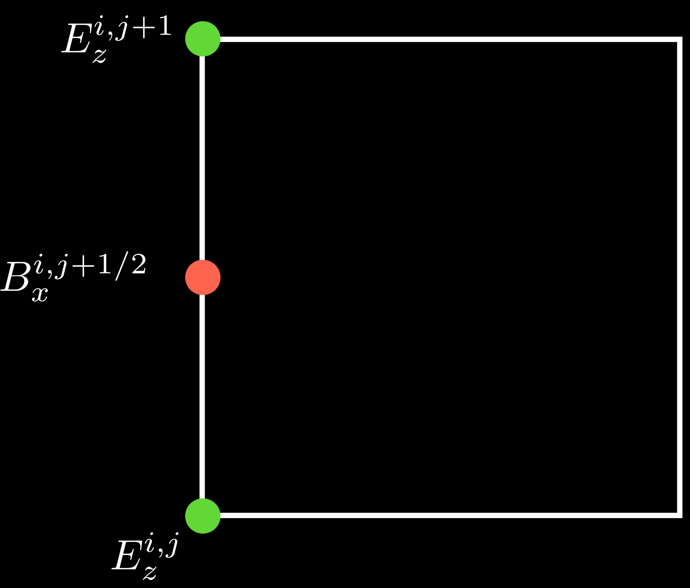
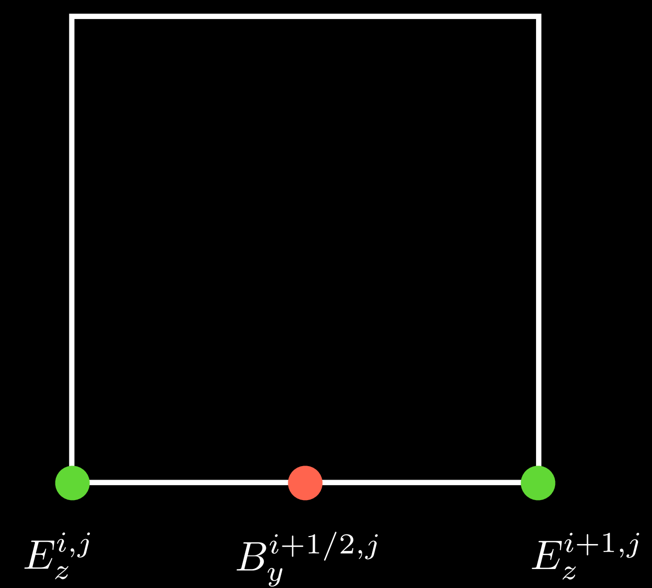
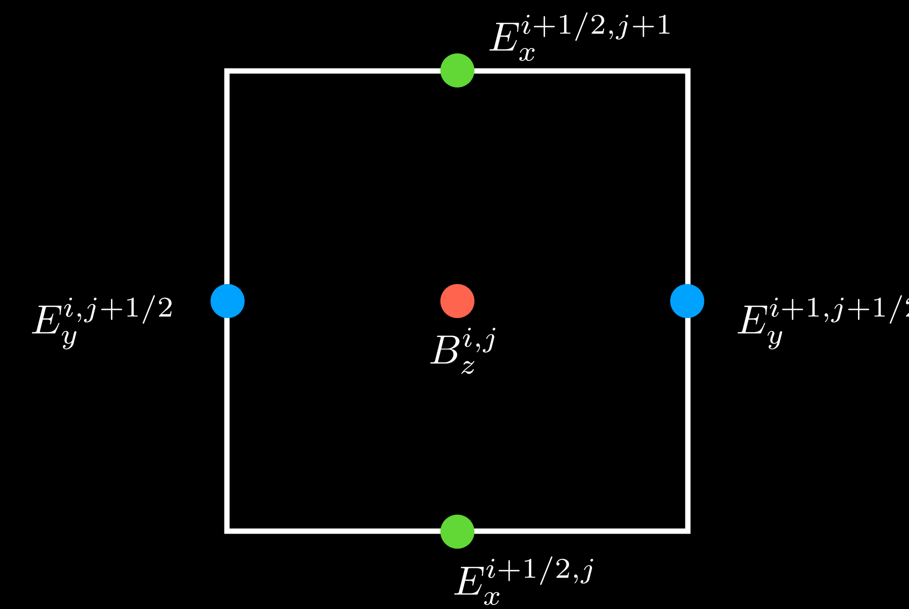
Why so (apparently) complicated?







$$\frac{\partial B_x}{\partial t} = -\frac{\partial E_z}{\partial y}$$

$$\frac{\partial B_y}{\partial t} = \frac{\partial E_z}{\partial x}$$

$$\frac{\partial B_z}{\partial t} = \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}$$

curl

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

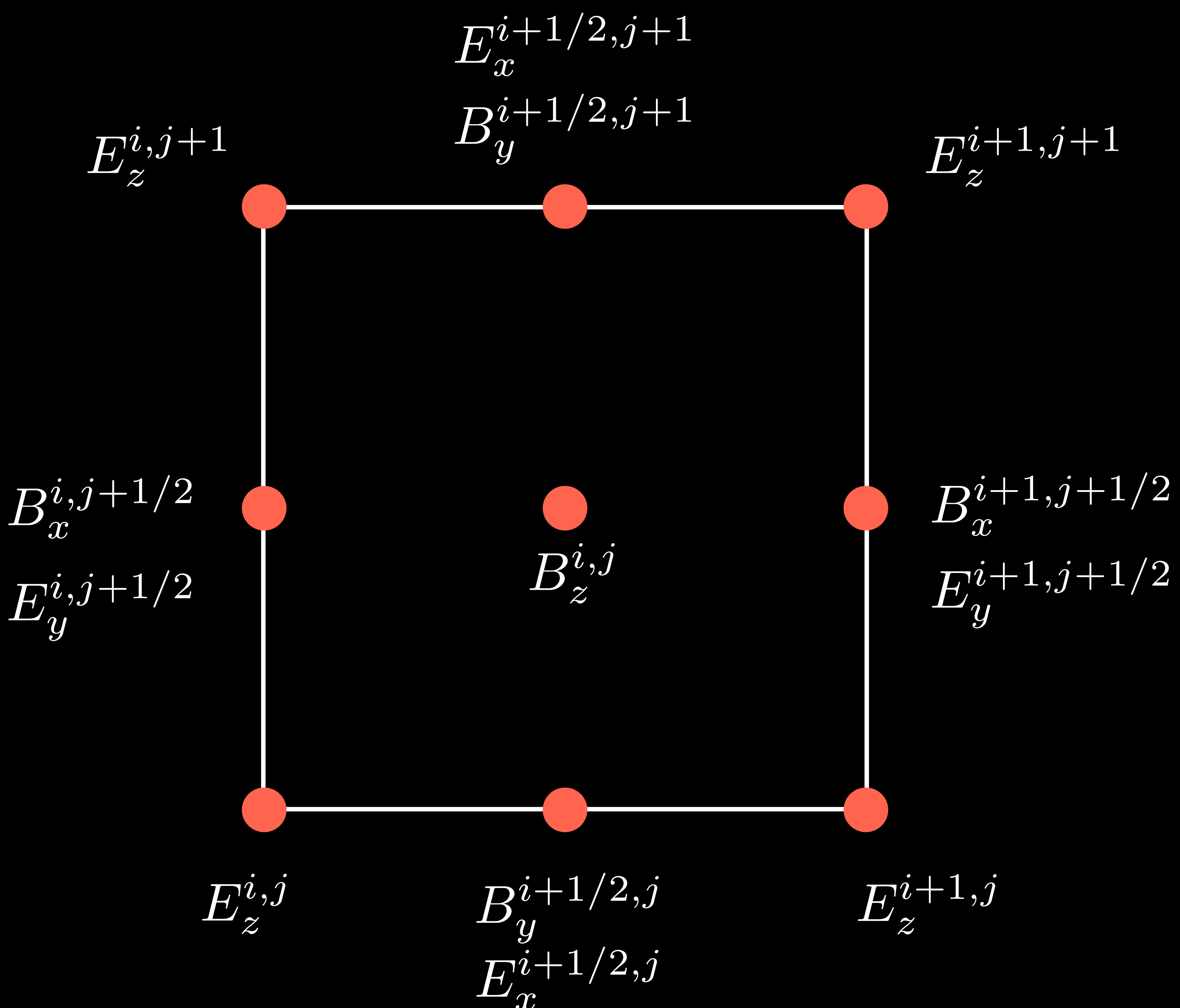
First order derivative

E and **B** components are positioned so to always have second order accurate finite difference approximation of the first order derivative

$$\frac{f_{i+1} - f_i}{\Delta x} = f'(x) + O(\Delta x)$$

$$\boxed{\frac{f_{i+1} - f_{i-1}}{2\Delta x} = f'(x) + O(\Delta x^2)}$$

Why so (apparently) complicated?



$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

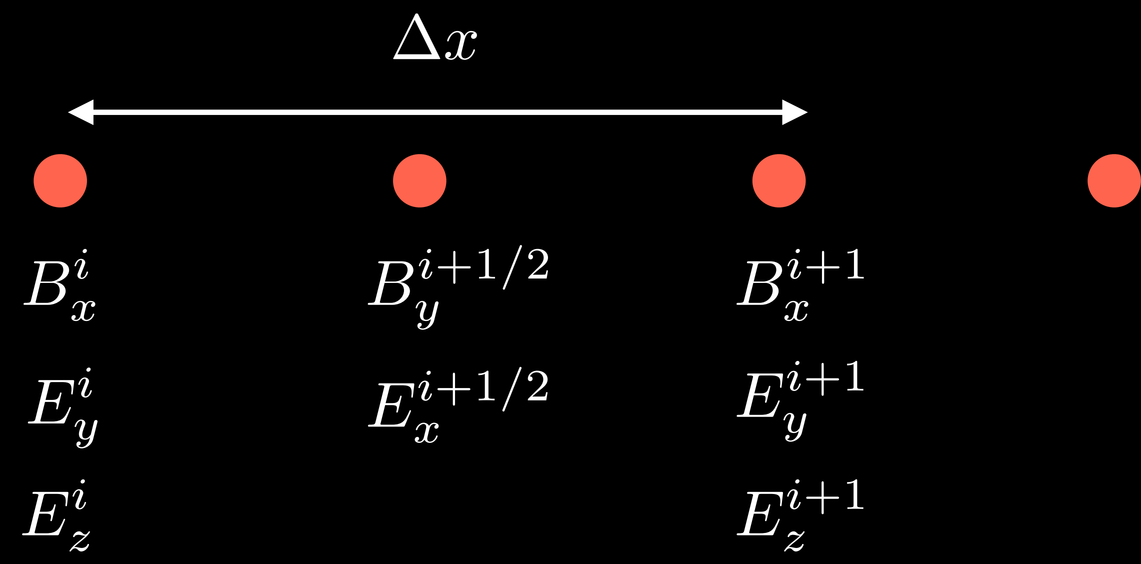
$$\frac{\partial \nabla \cdot \mathbf{B}}{\partial t} = -\nabla \cdot \nabla \times \mathbf{E} = 0$$

Maxwell-Faraday equation conserves $\nabla \cdot \mathbf{B} = 0$

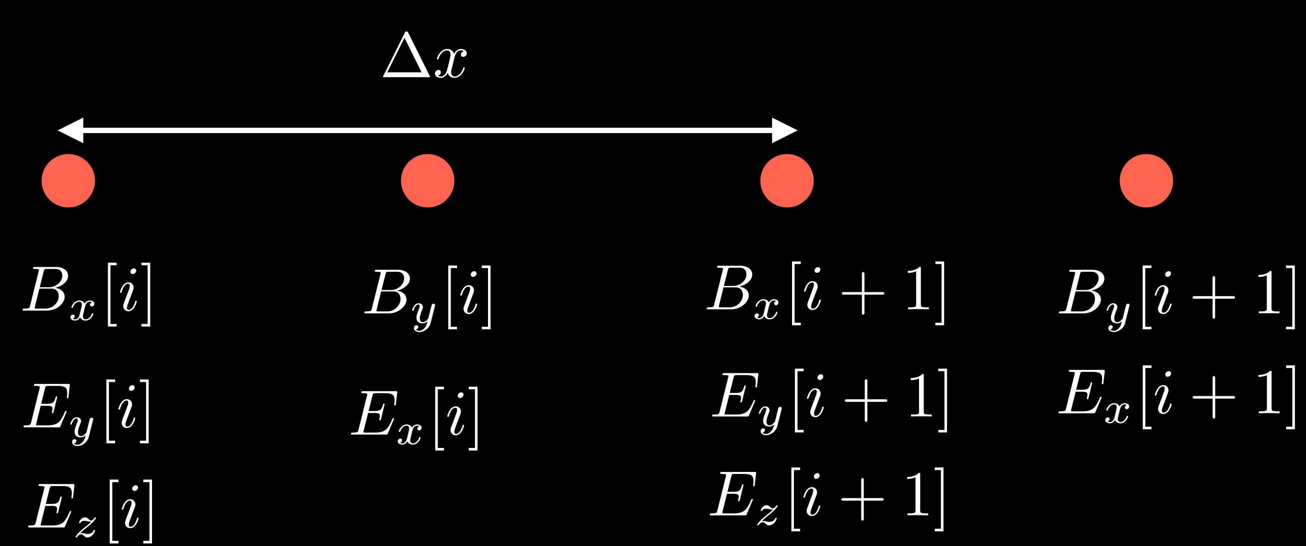
The Yee mesh conserves the discrete divergence to 0 at machine precision

Tips: write the discrete version of $\frac{\partial \nabla \cdot \mathbf{B}}{\partial t} = -\nabla \cdot \nabla \times \mathbf{E} = 0$

FROM MATH TO ARRAYS



In practice arrays only have integer indices



Hands on!

Boris

Hands on drifts