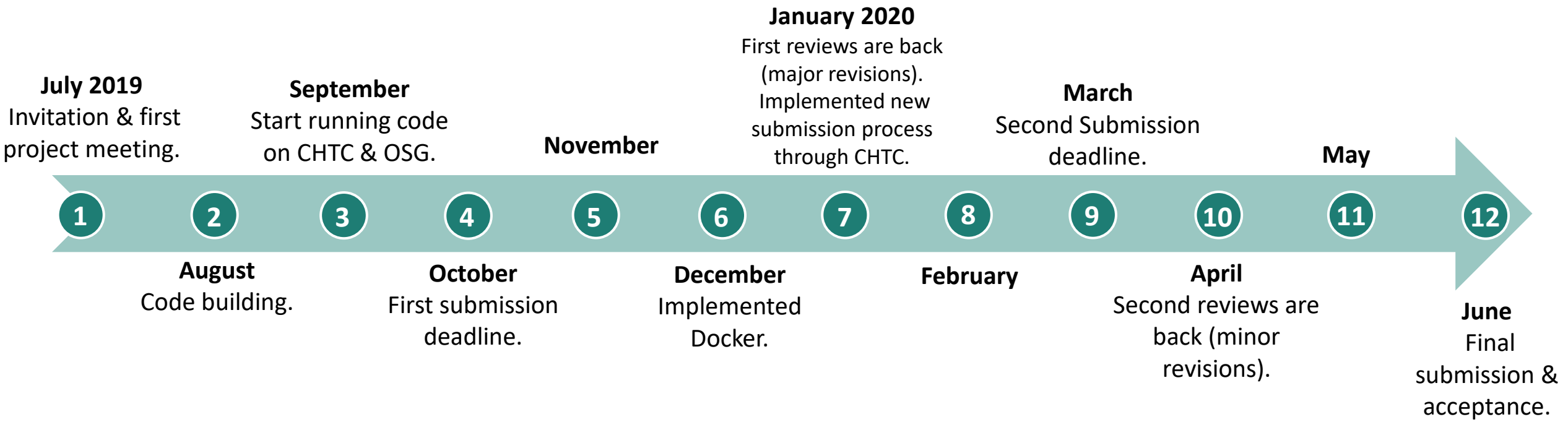
OSG resources enable optimization of field experimental designs for agriculture

OSG All-Hands Meeting 2020

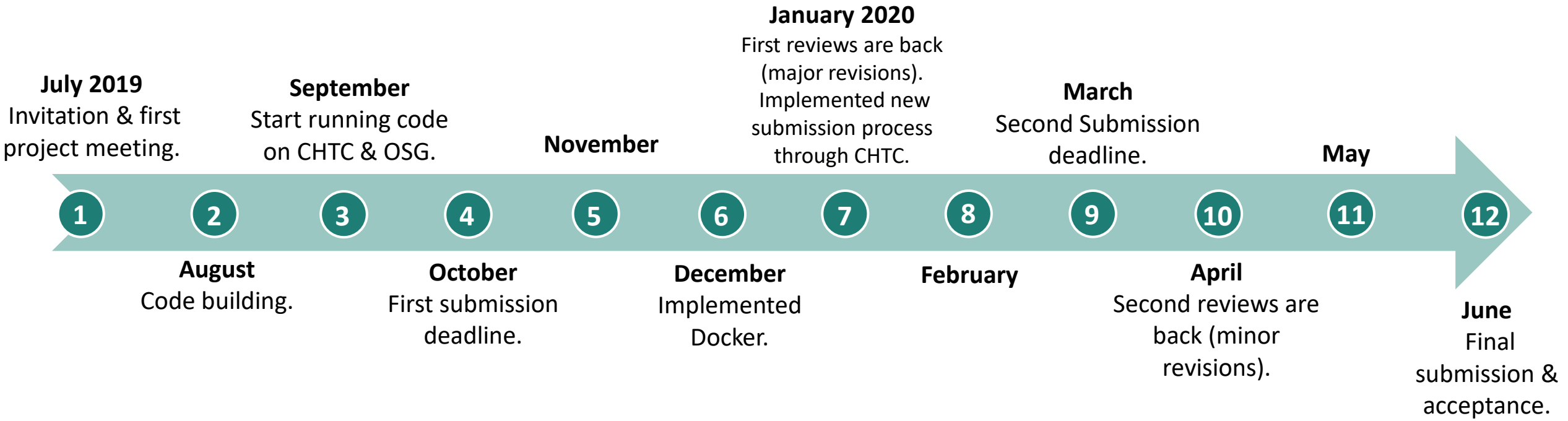
Cereals Breeding and Quantitative Genetics
University of Wisconsin-Madison

Raegan Hoefler, Pablo Gonzalez-Barrios, Madhav Bhatta, Jose A. R. Nunes, Ines Berro, Rafael S. Nalin, Alejandra Borges, Eduardo Covarrubias, Luis Diaz-Garcia, Martin Quincke, Lucia Gutierrez

Overview

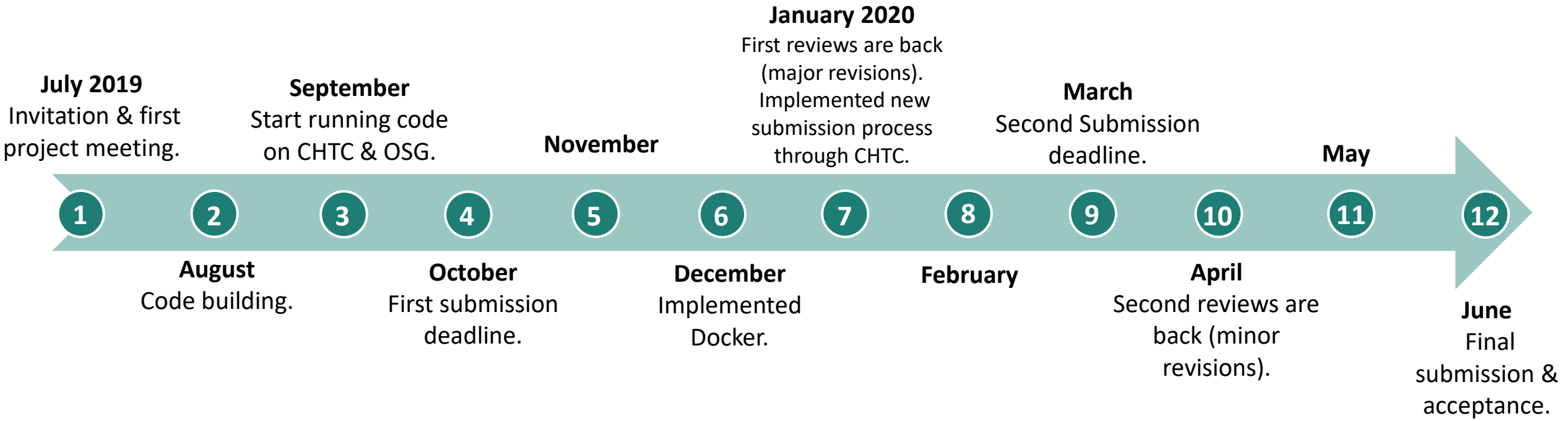

July 2019
Invitation & first project meeting.
August
Code building.
September
Start running code on CHTC & OSG.
October
First submission deadline.
November
December
Implemented Docker.
January 2020
First reviews are back (major revisions). Implemented new submission process through CHTC.
February
March
Second Submission deadline.
April
Second reviews are back (minor revisions).
May
June
Final submission & acceptance.
1
2
3
4
5
6
7
8
9
10
11
12

Overview



3.73 M hours through OSG Connect

Overview



3.73 M hours through OSG Connect
+ 533,000 hours through OSG via CHTC

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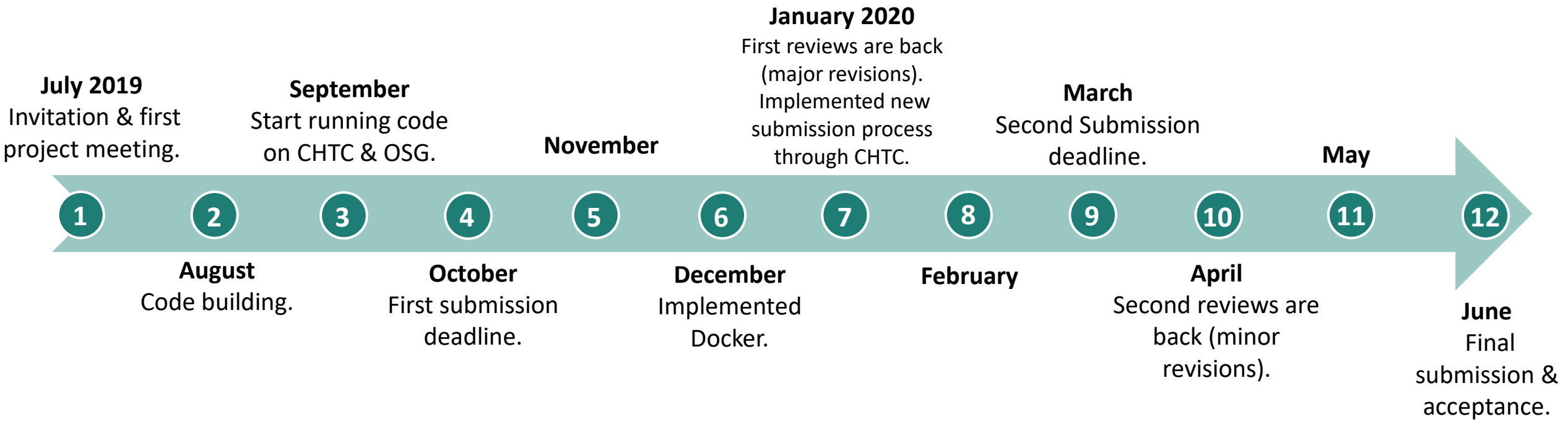

3.73 M hours through OSG Connect
+ 533,000 hours through OSG via CHTC
+ 1.8 M hours through CHTC

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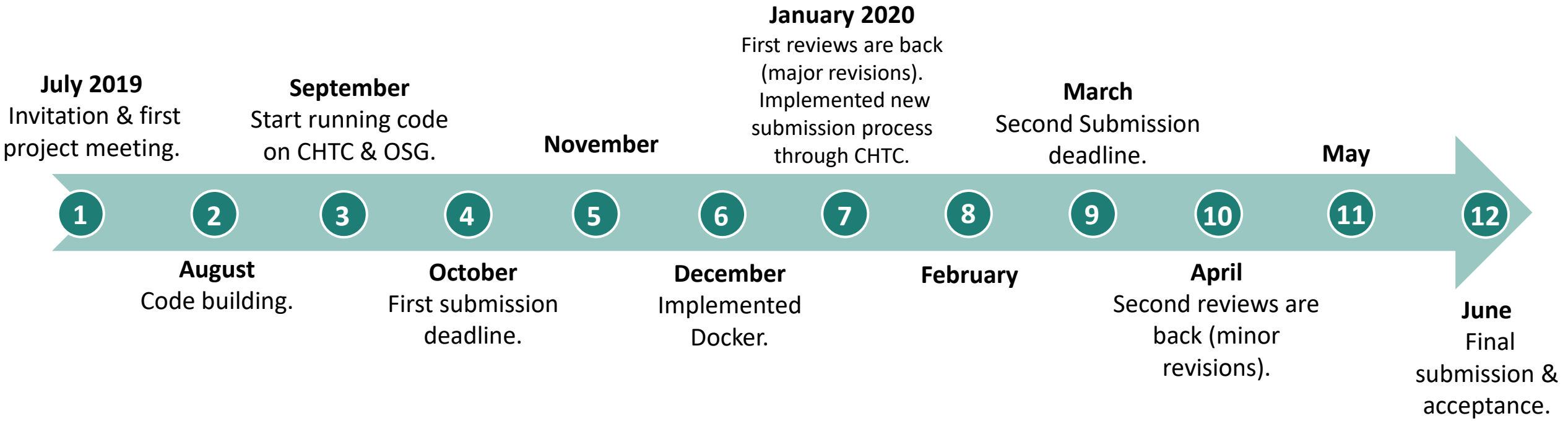
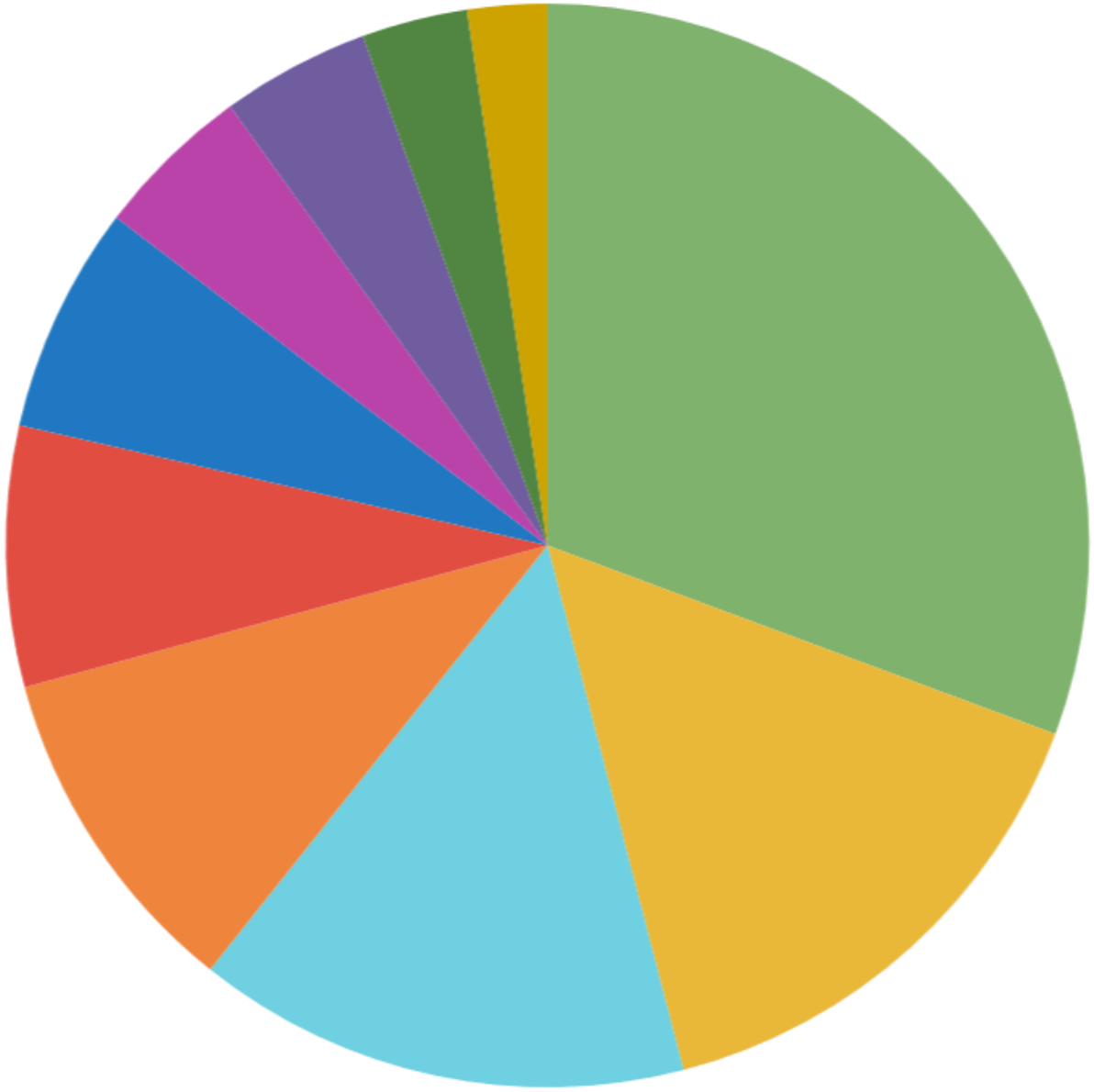


3.73 M hours through OSG Connect
+ 533,000 hours through OSG via CHTC
+ 1.8 M hours through CHTC

= 6 M hours (many triumphs, many fails)

Overview



OSG Connect Summary:
Total Wall Hours for Top 10 Projects
July 1, 2019 - June 30, 2020

https://gracc.opensciencegrid.org/d/000000099/osg-connect-summary-osgconnect-net-submit-hosts-only?orgId=1&from=1561939200000&to=1593561599000&var-interval=1d&var-project=All&var-user=All&var-Filter=ProbeName%7C%3D~%7C.*osgconnect%5C.net

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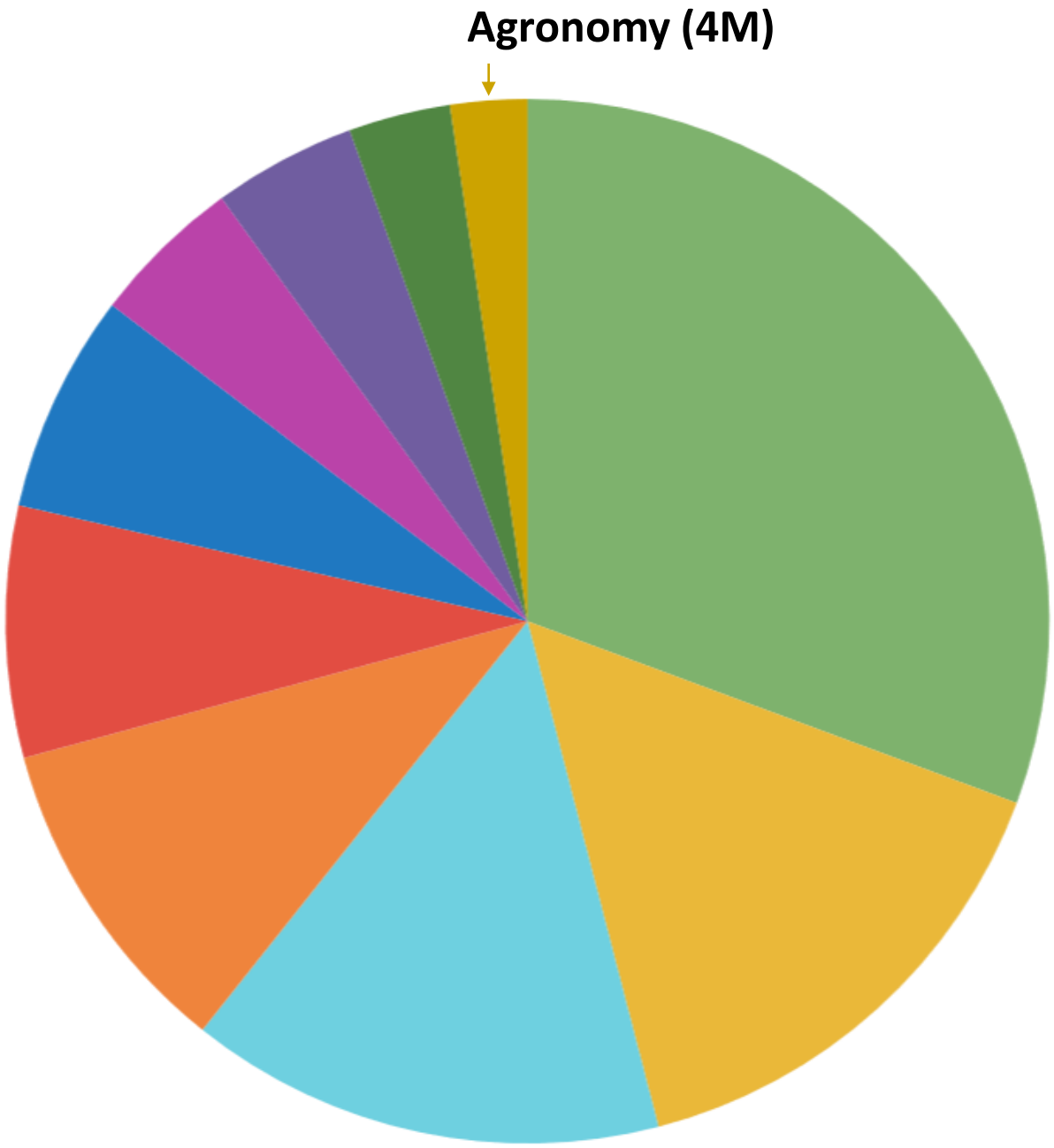

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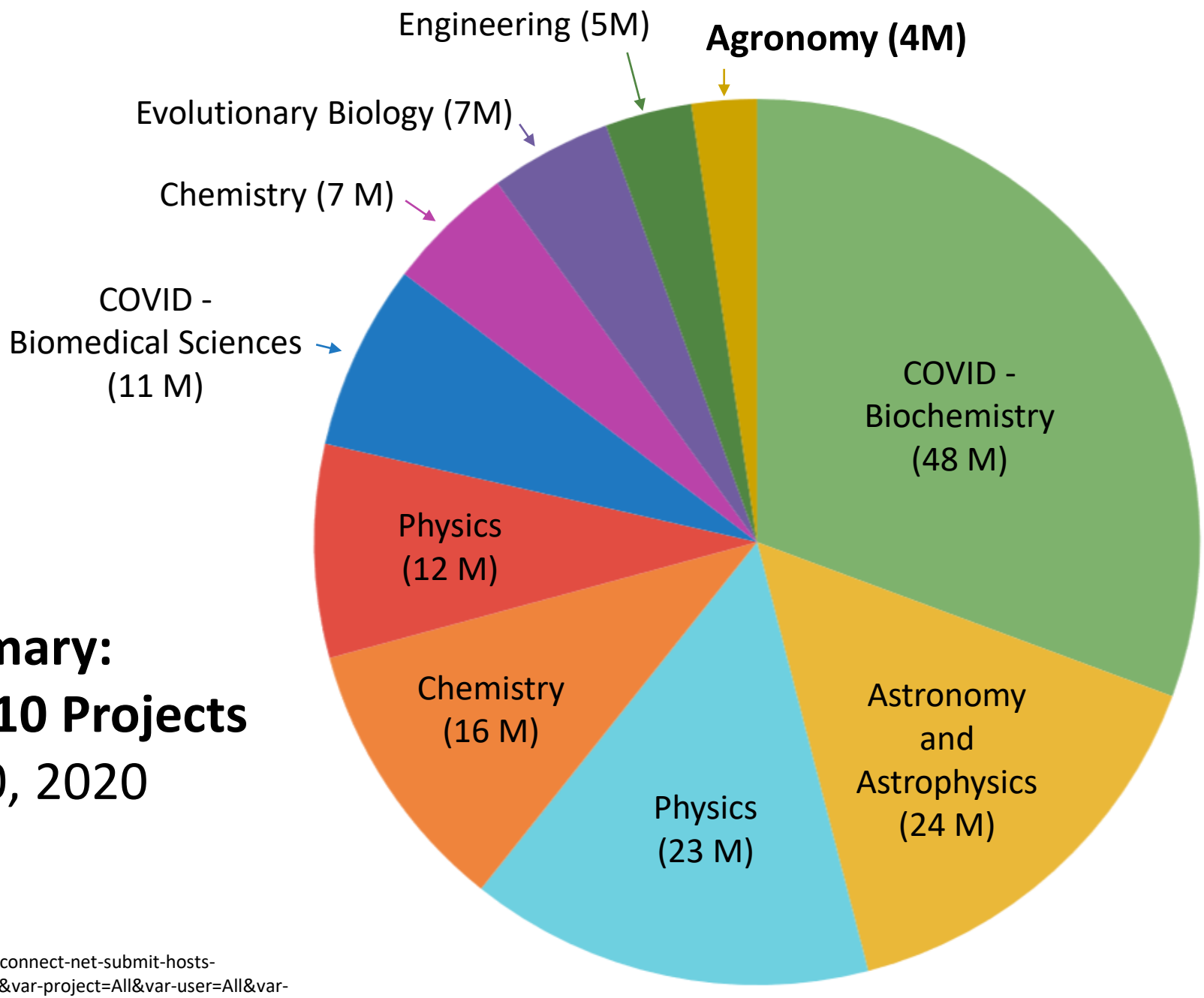

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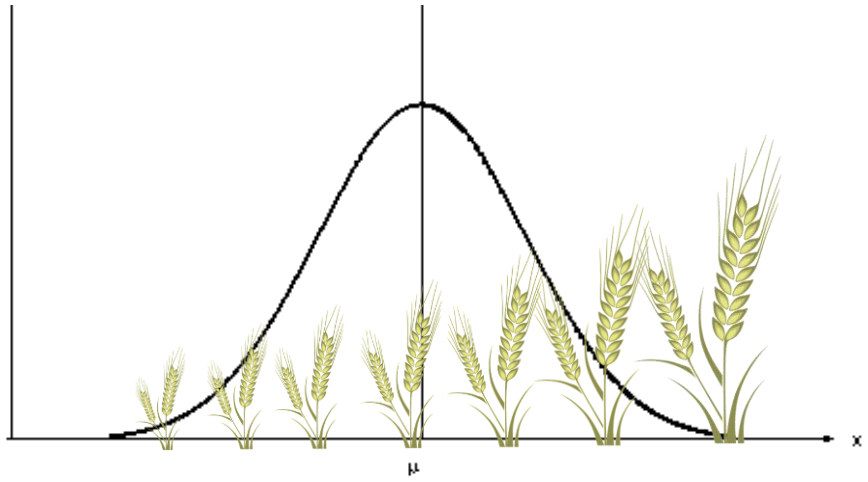
- Our areas of research: experimental design optimization for genomic studies and modeling genotype by environment interactions
- Invited paper: Journal of Agricultural Biological and Environmental Statistics (JABES)
  - Questions of interest:
    1. Do spatial designs outcompete randomization-based designs?
    2. Do additional methods of spatial correction help?

Background: Response to Selection

Parents



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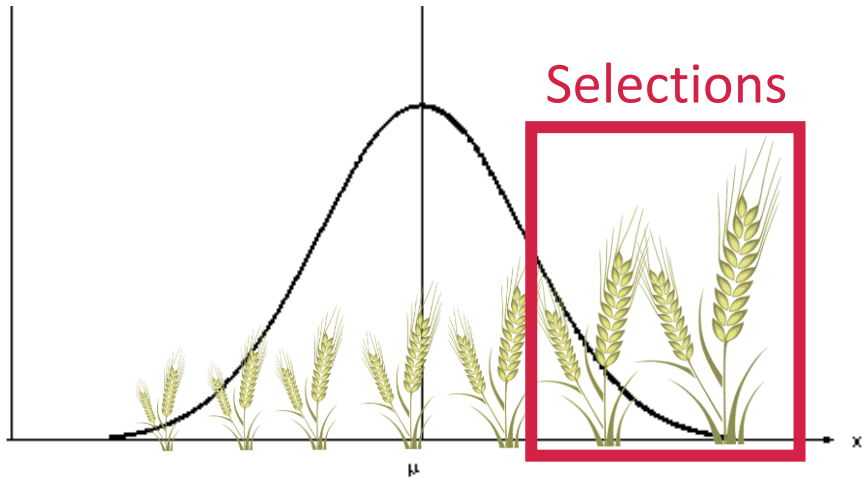

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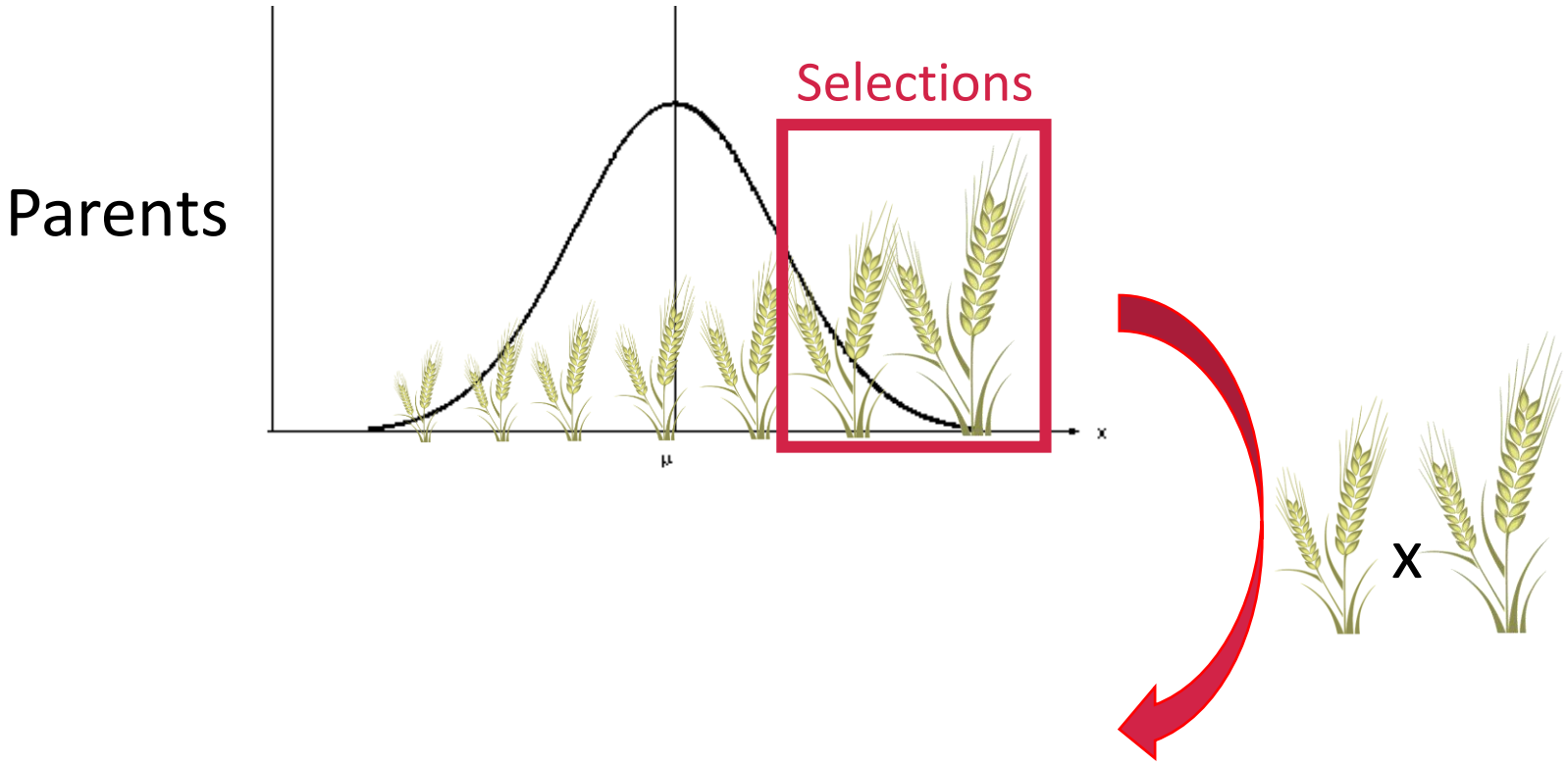

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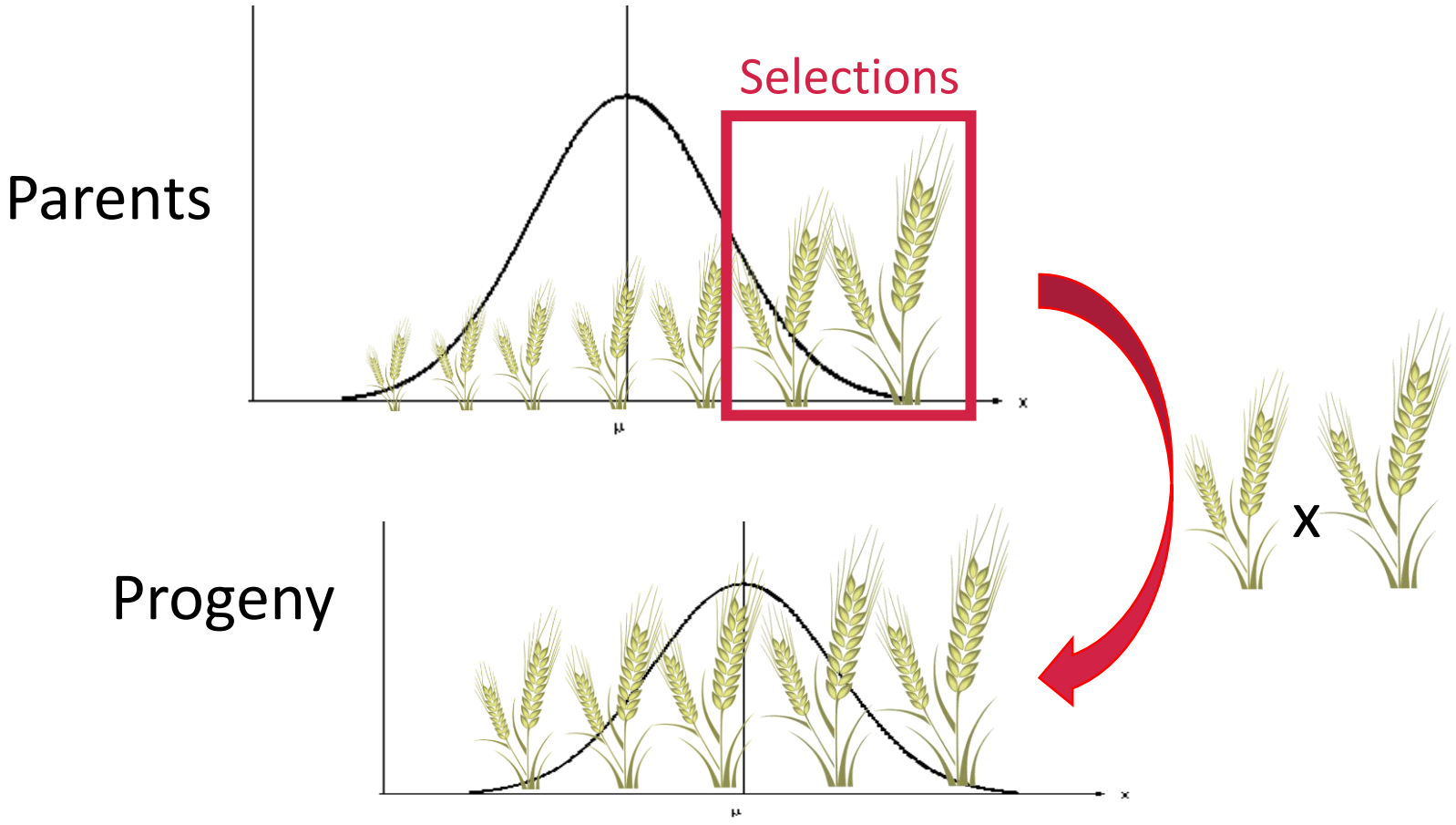

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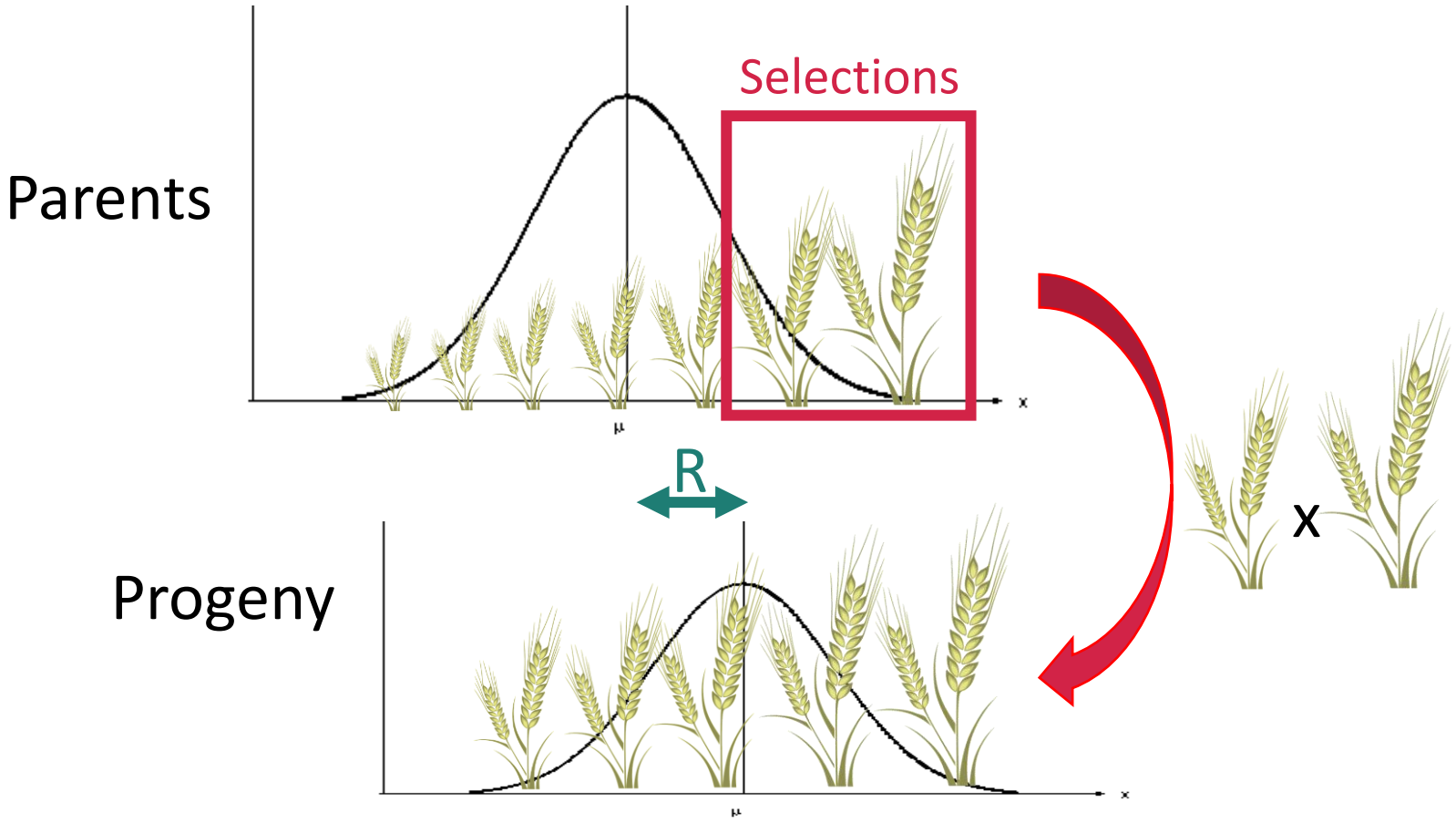

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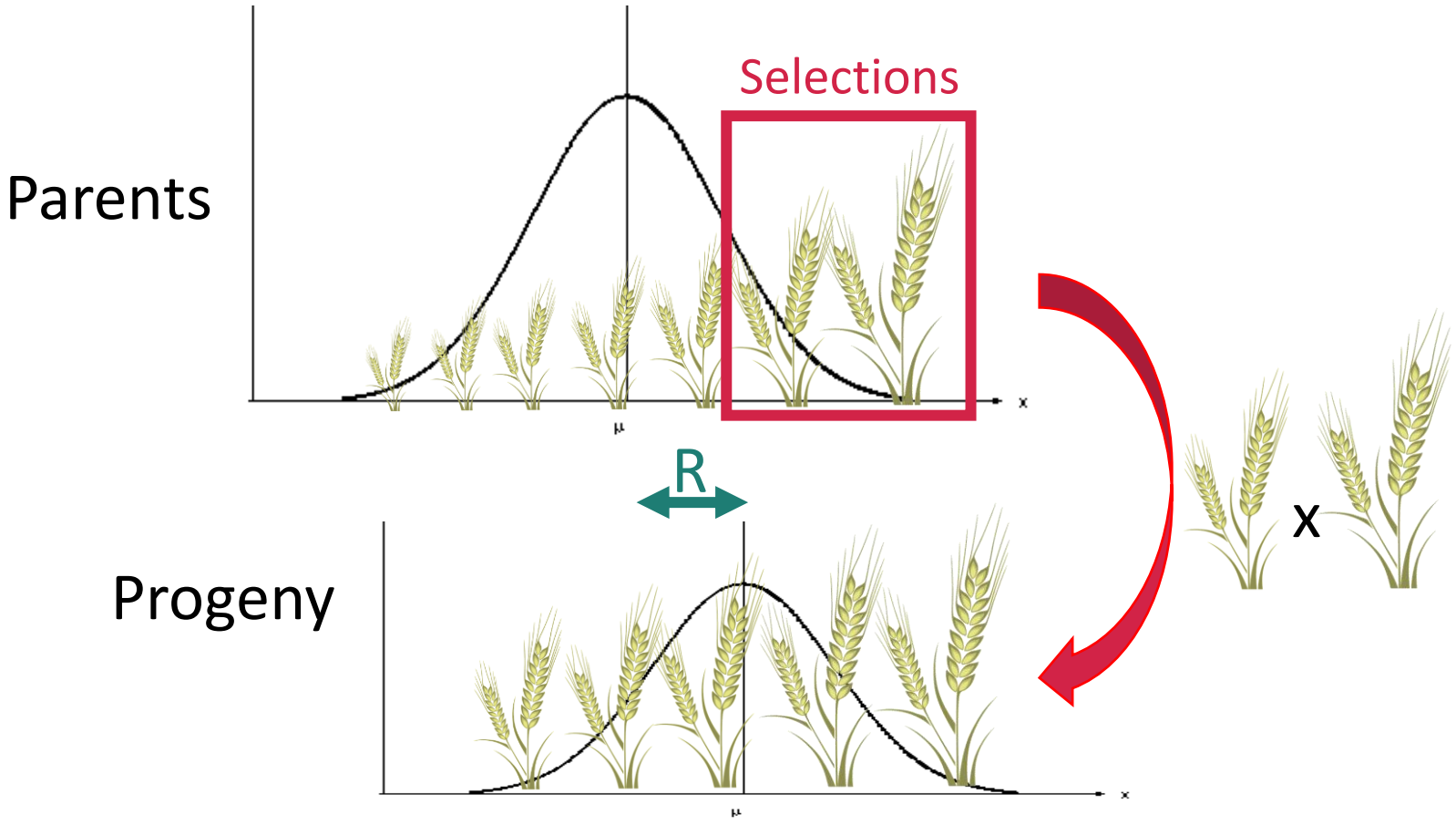

"Breeder's Equation"

$$R = ir_{g,\hat{g}}\sigma_g$$

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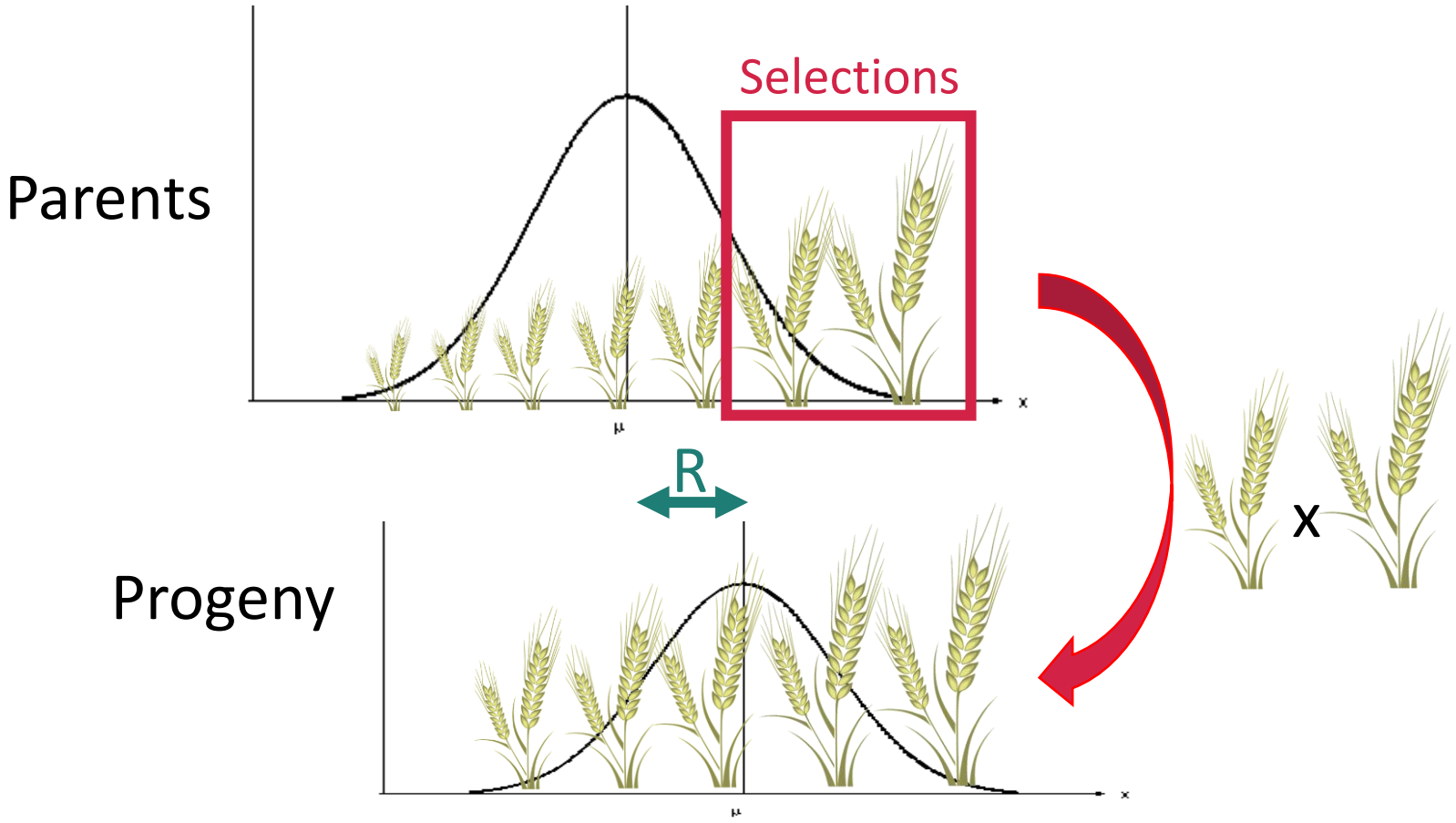

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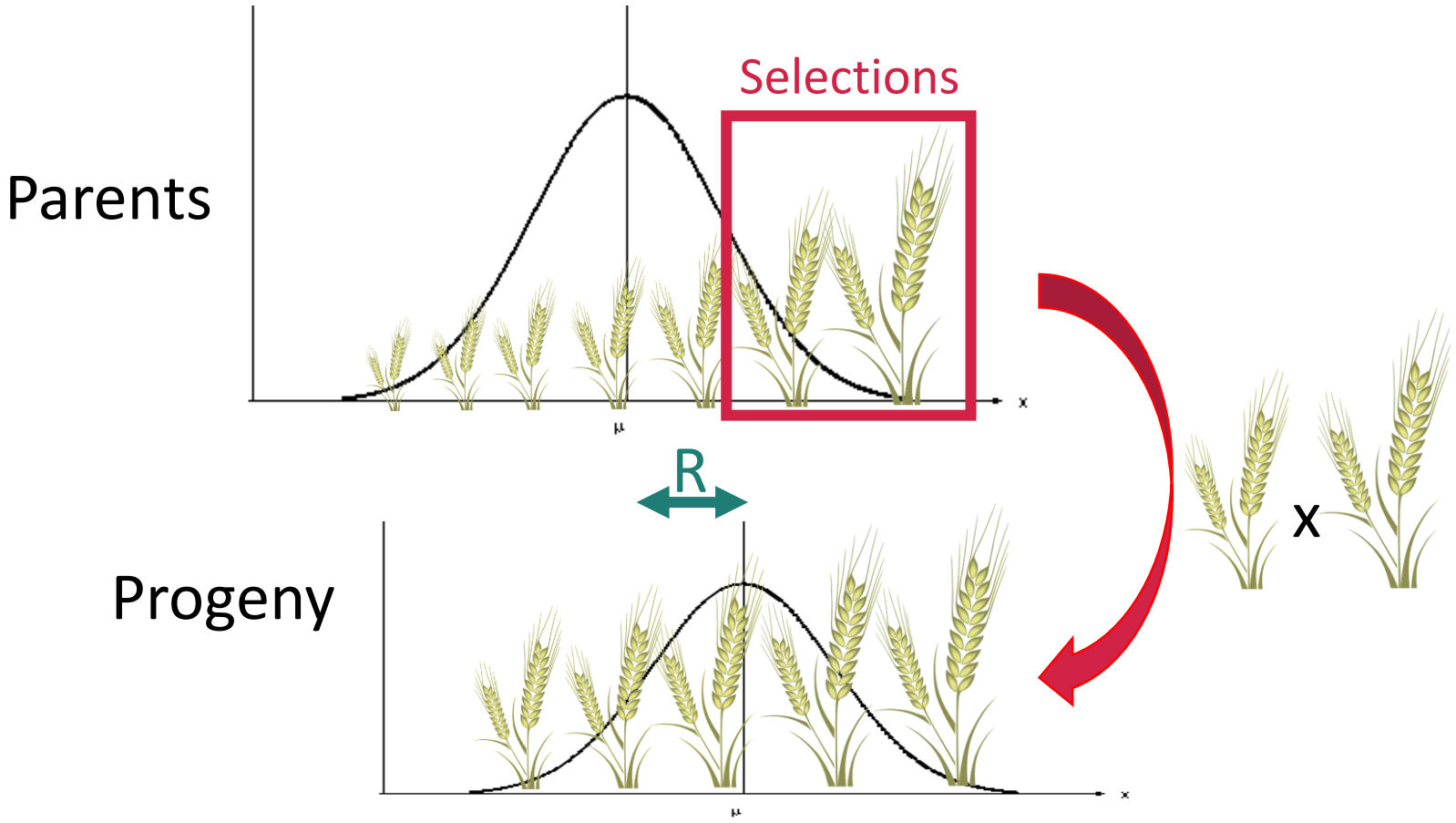

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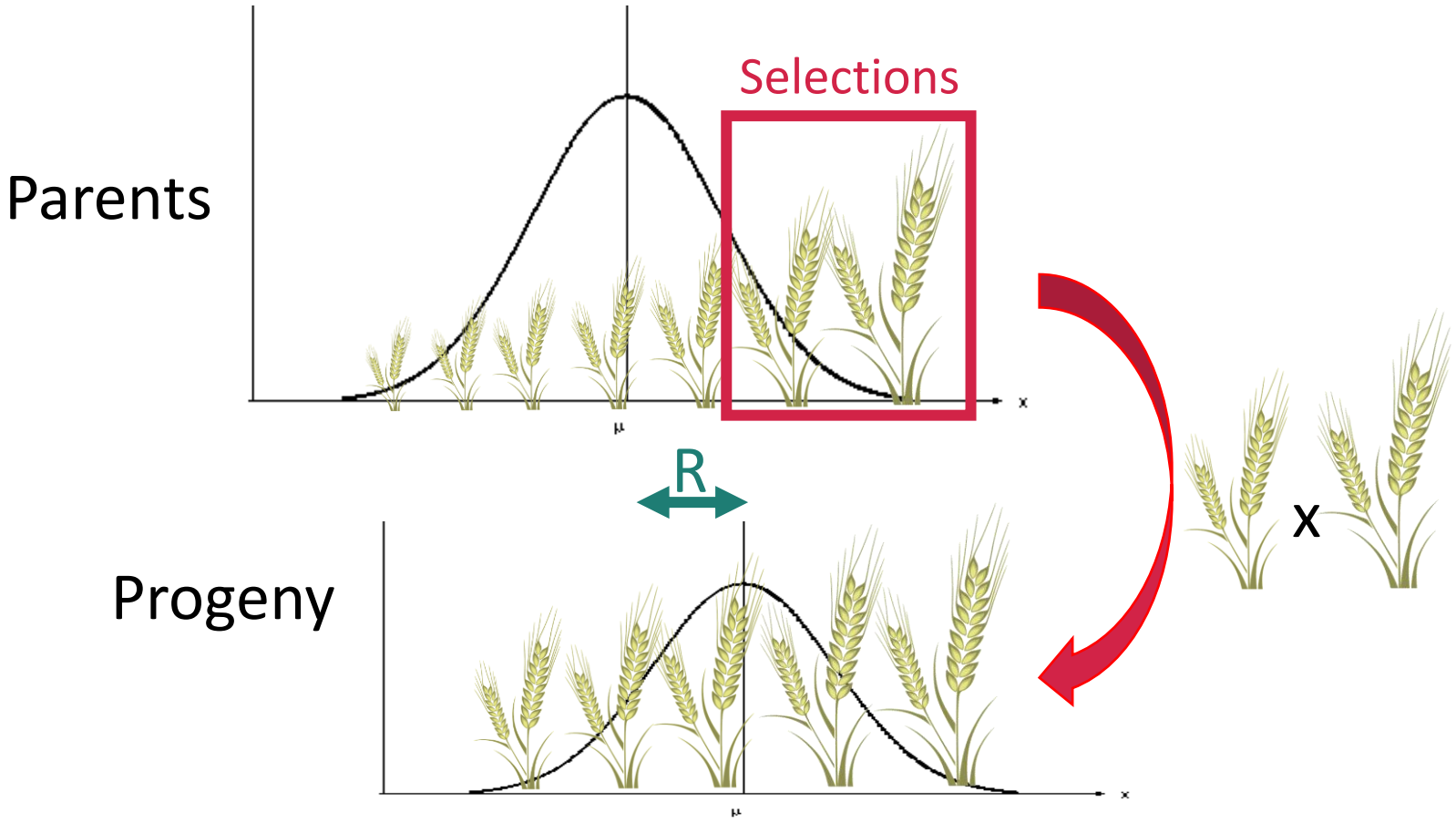
True (g)

Background: Response to Selection



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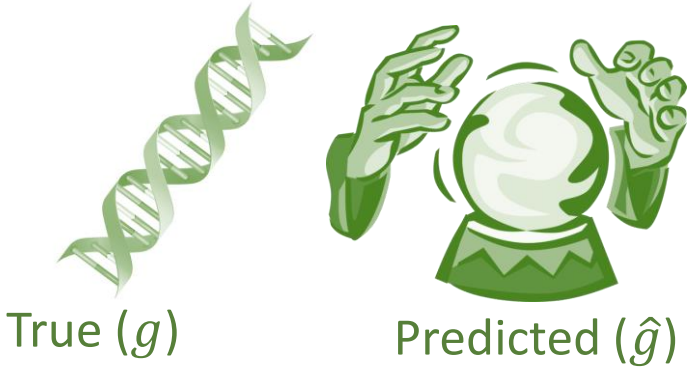

Background: Spatial Variation

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Must control spatial variation!

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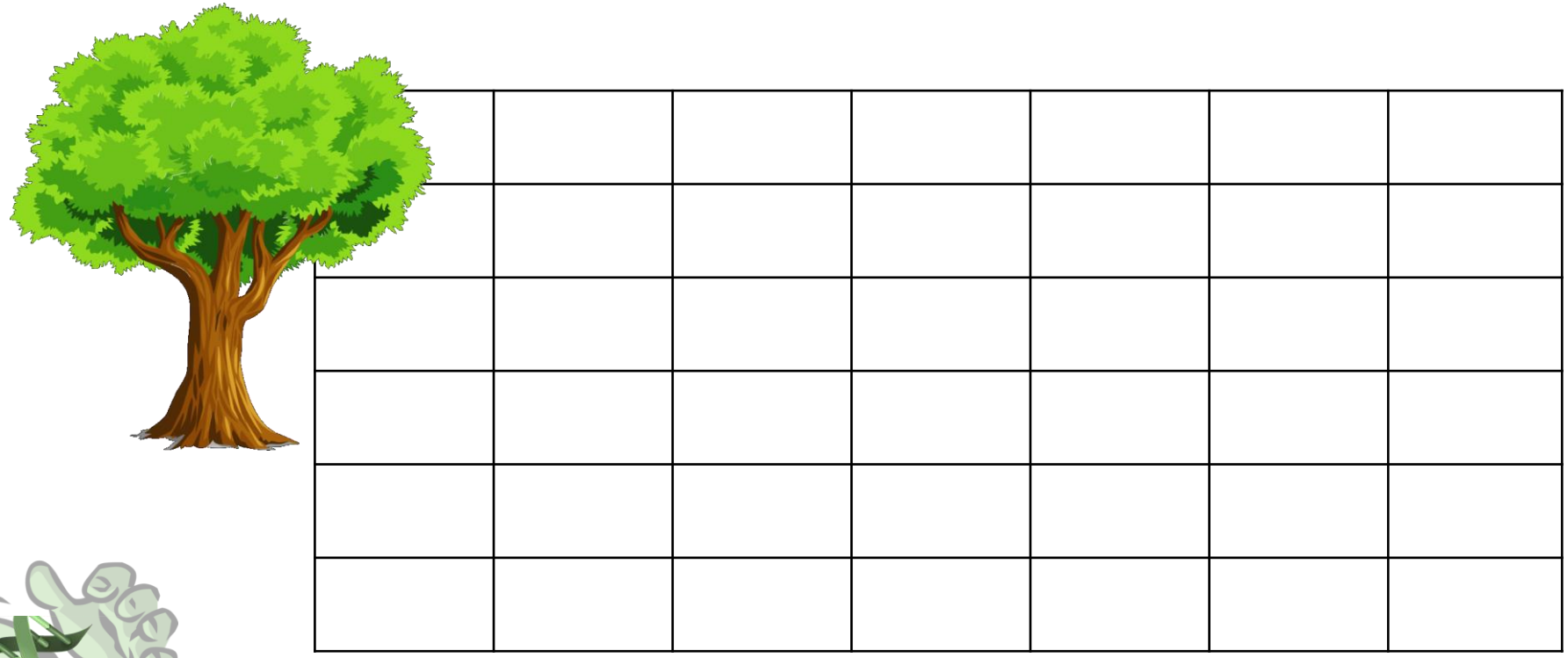

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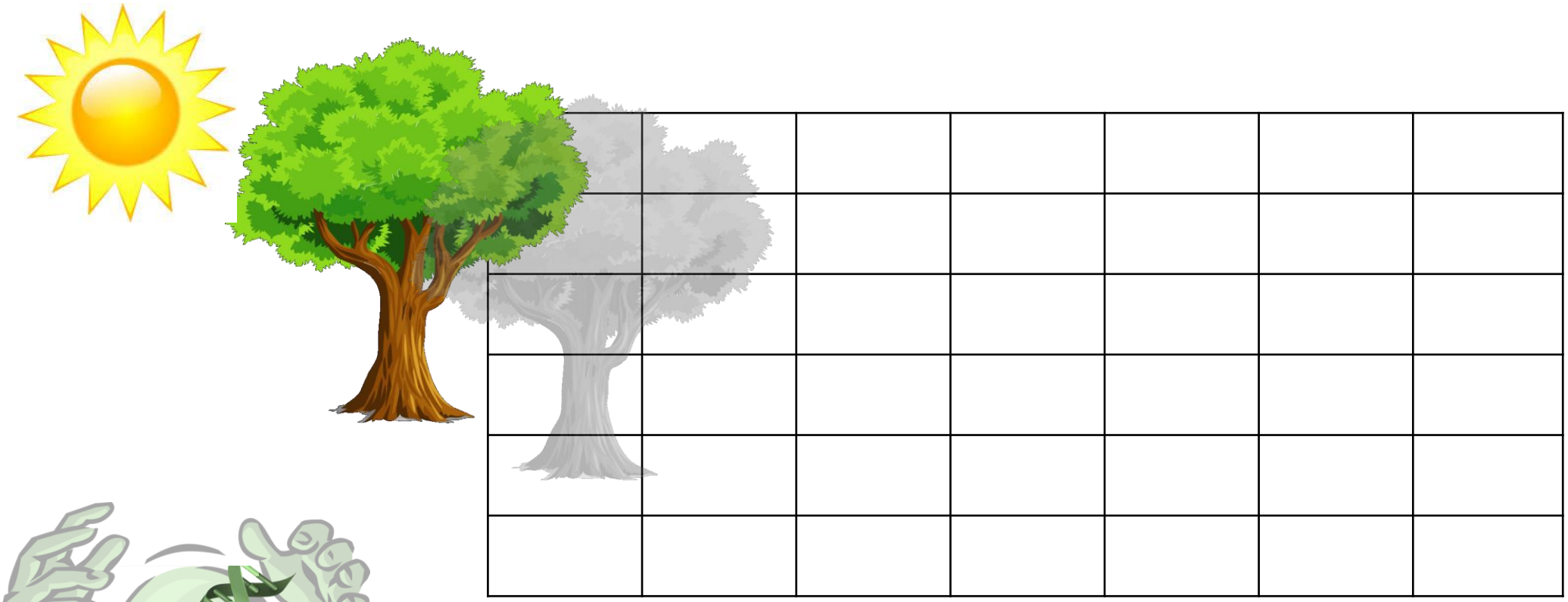

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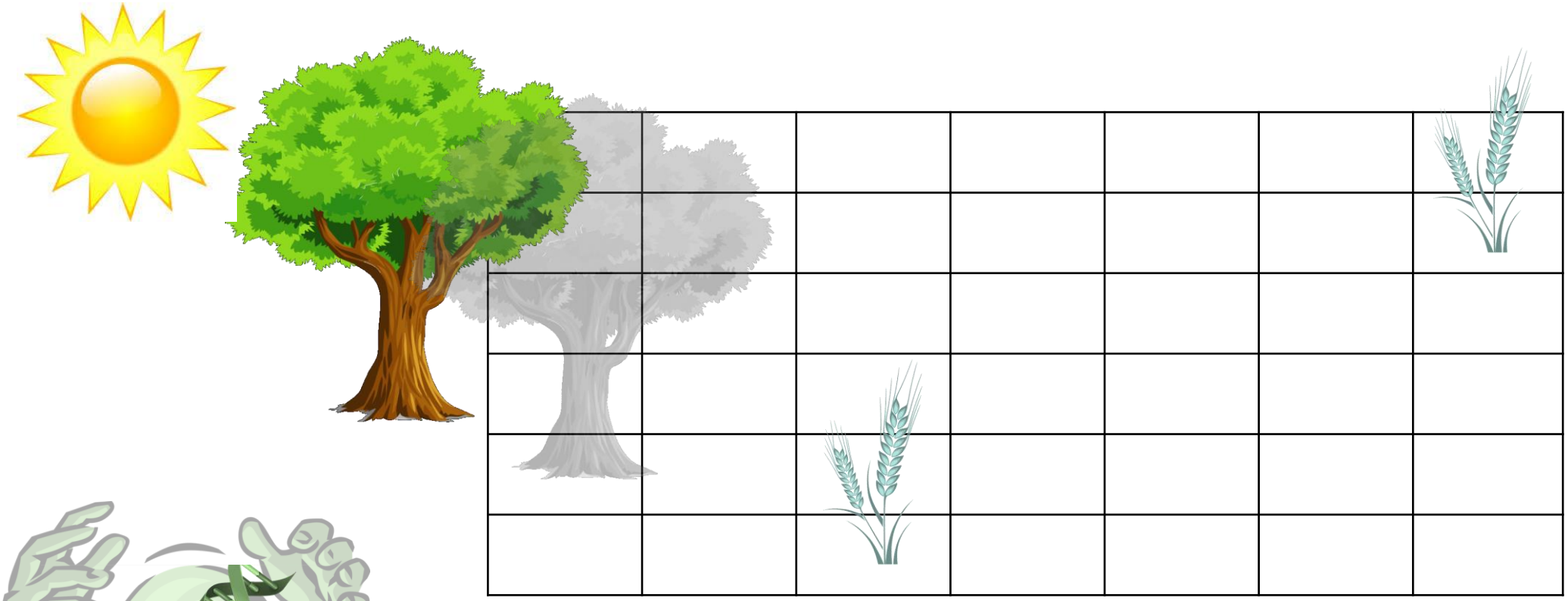

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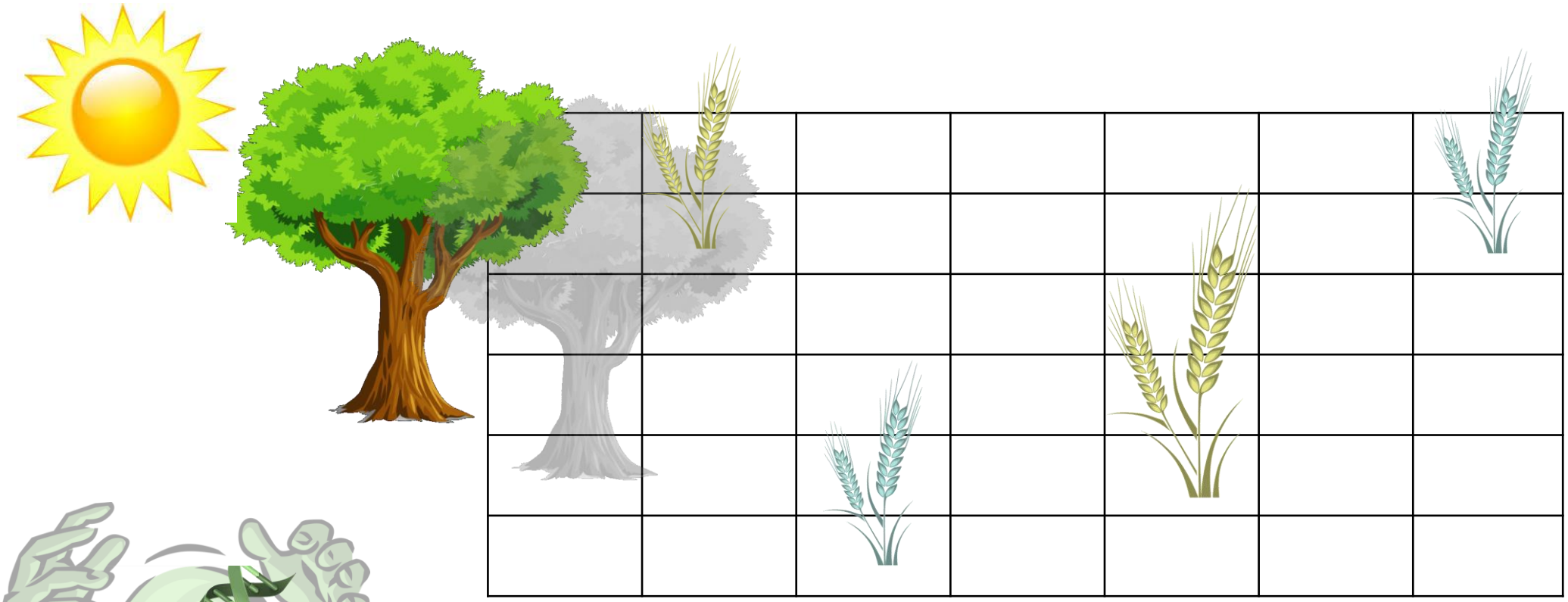
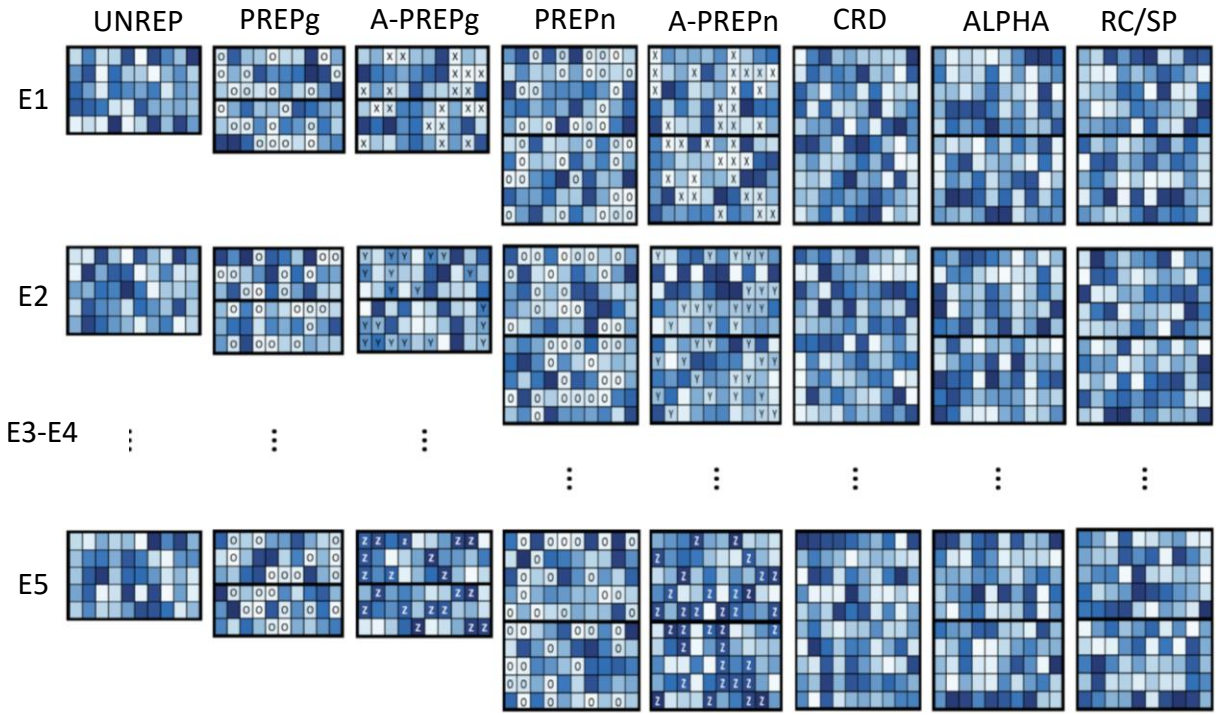


Must control spatial variation!

Background: Experimental Design

Design

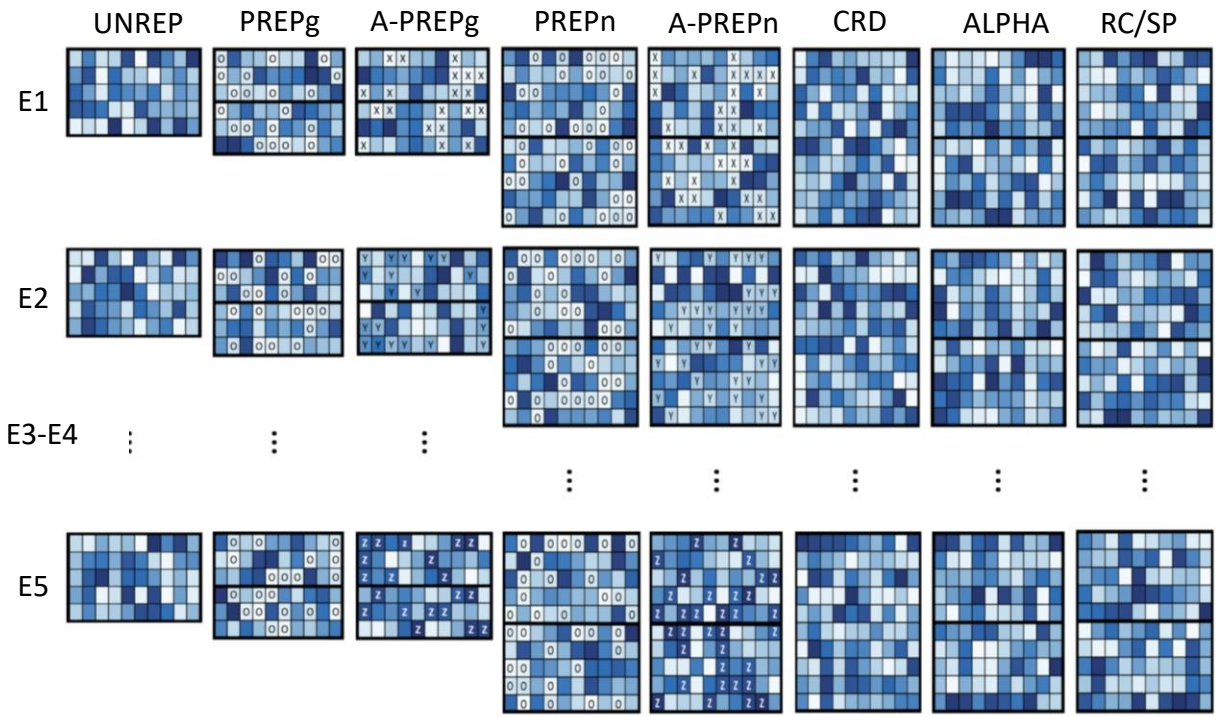


-How many genotypes?
-How many plots?

-How many replicated?
-How many environments?

Background: Experimental Design

Design



-How many genotypes?
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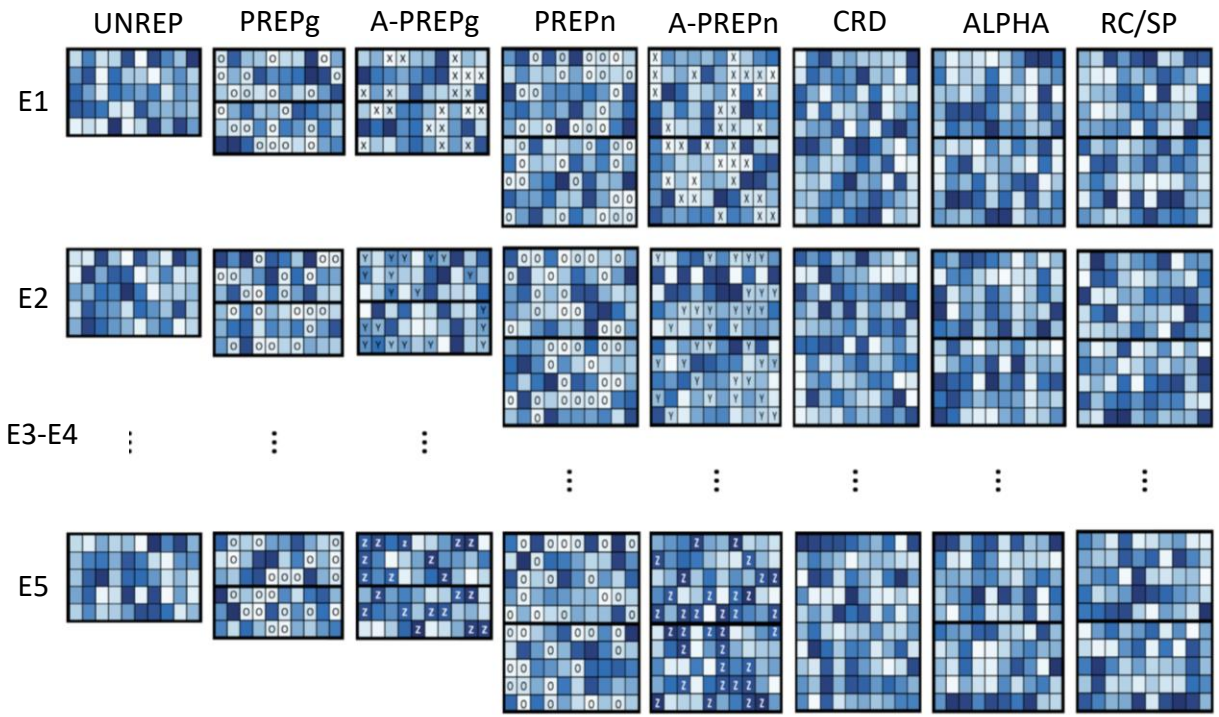
Evaluate

- Labor
- Time

Background: Experimental Design

Design



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-How many environments?

Evaluate

- Labor
- Time

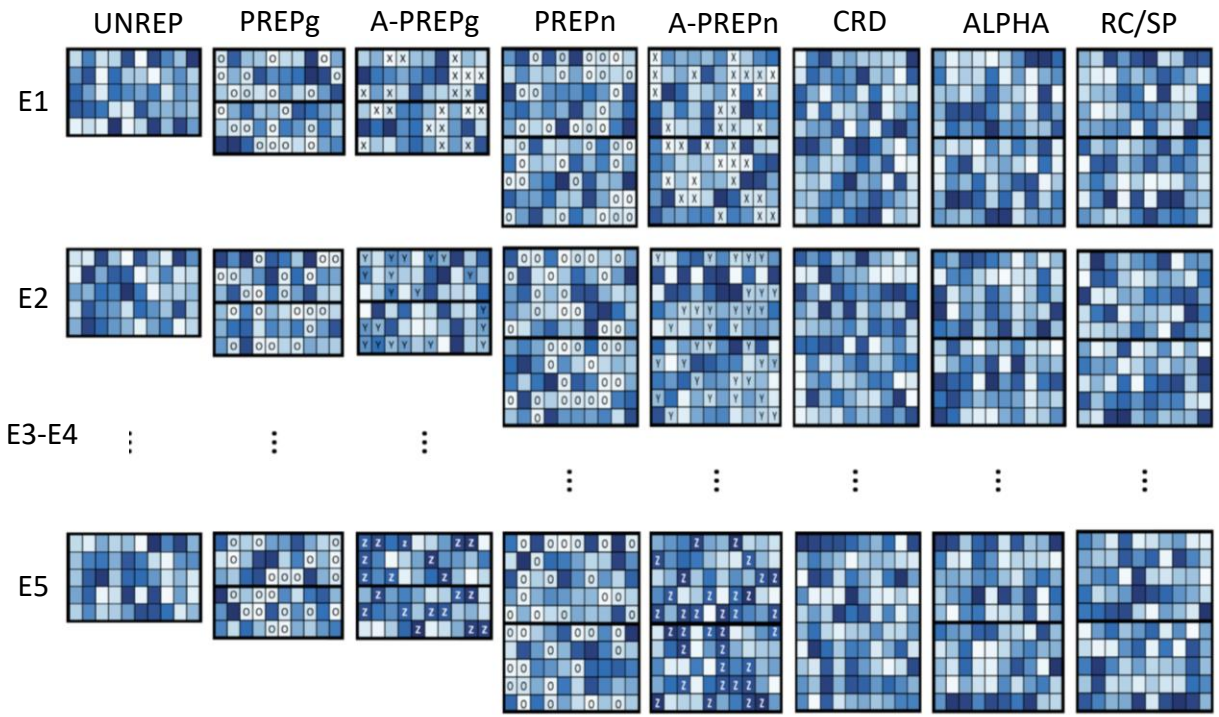
Analyze

$$y_{ijklm} = \mu + \hat{g}_i + e_j + ge_{ij} + D_{k(j)} + S_{lm(j)} + \varepsilon_{ijklm}$$

$$yield = mean + \hat{g}_i + \text{env} + \text{GE} + \text{design} + \text{spatial} + \text{error}$$

Background: Experimental Design

Design



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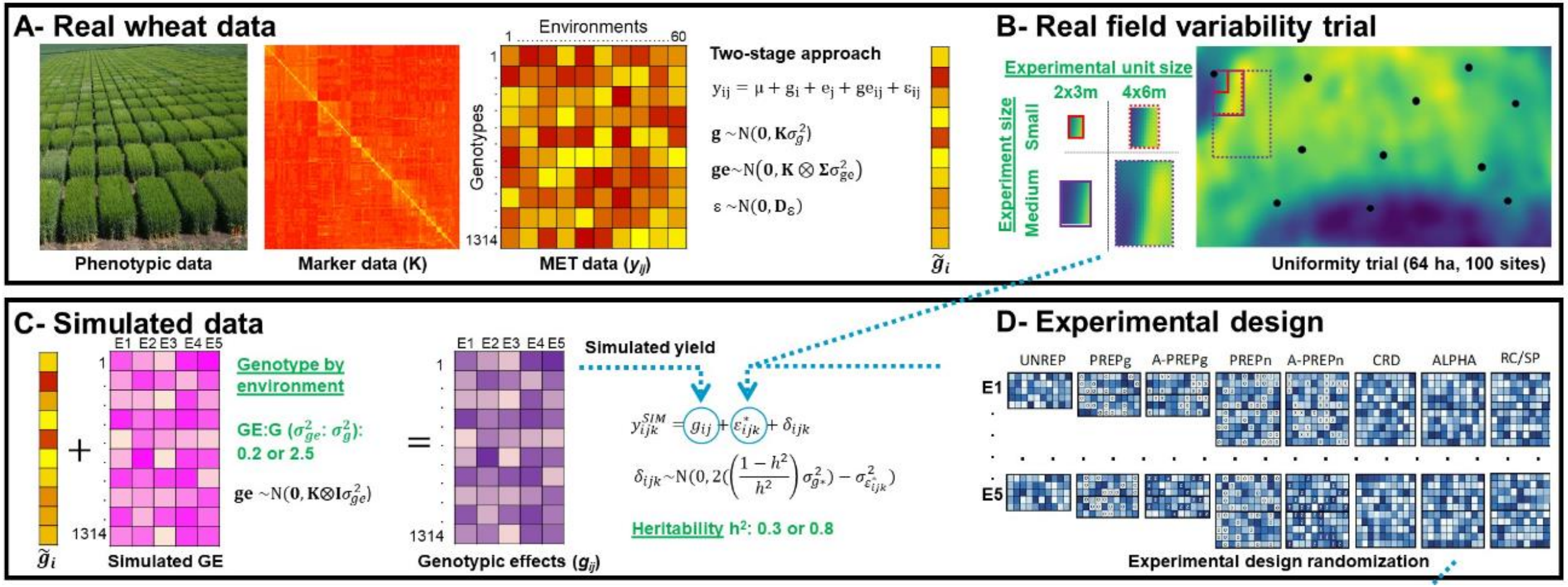
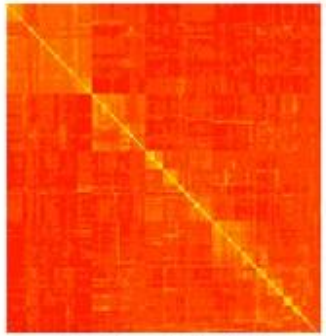
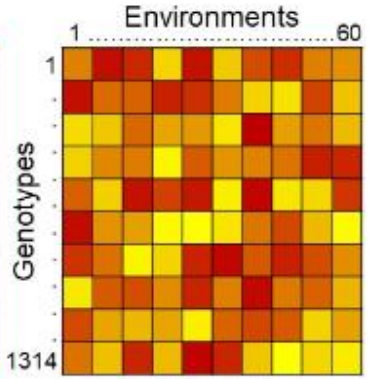

A- Real wheat data
Phenotypic data
Marker data (K)
Environments
1
60
Genotypes
1
1314
MET data (y_{ij})
Two-stage approach
$y_{ij} = \mu + g_i + e_j + ge_{ij} + \varepsilon_{ij}$
$g \sim N(0, K\sigma_g^2)$
$ge \sim N(0, K \otimes \Sigma\sigma_{ge}^2)$
$\varepsilon \sim N(0, D_\varepsilon)$
$\tilde{g}_i$
B- Real field variability trial
Experimental unit size
2x3m
4x6m
Experiment size
Small
Medium
Uniformity trial (64 ha, 100 sites)
C- Simulated data
E1 E2 E3 E4 E5
1
1314
$\tilde{g}_i$
Simulated GE
Genotype by environment
GE:G (σ_{ge}^2: σ_g^2): 0.2 or 2.5
$ge \sim N(0, K \otimes I\sigma_{ge}^2)$
Genotypic effects (g_{ij})
Simulated yield
$y_{ijk}^{SIM} = g_{ij} + \varepsilon_{ijk}^* + \delta_{ijk}$
$\delta_{ijk} \sim N(0, 2(\left(\frac{1-h^2}{h^2}\right)\sigma_{g*}^2) - \sigma_{\varepsilon_{ijk}^*}^2)$
Heritability h^2: 0.3 or 0.8
D- Experimental design
UNREP
PREPg
A-PREPg
PREPn
A-PREPn
CRD
ALPHA
RC/SP
E1
E5
Experimental design randomization

A- Real wheat data

Phenotypic data



Marker data (K)



MET data (y_{ij})

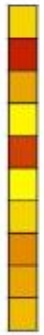
Two-stage approach

$$y_{ij} = \mu + g_i + e_j + ge_{ij} + \varepsilon_{ij}$$

$$\mathbf{g} \sim N(\mathbf{0}, \mathbf{K}\sigma_g^2)$$

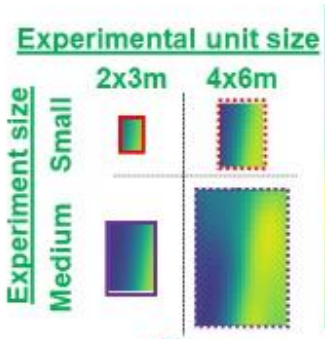
$$\mathbf{ge} \sim N(\mathbf{0}, \mathbf{K} \otimes \mathbf{\Sigma}\sigma_{ge}^2)$$

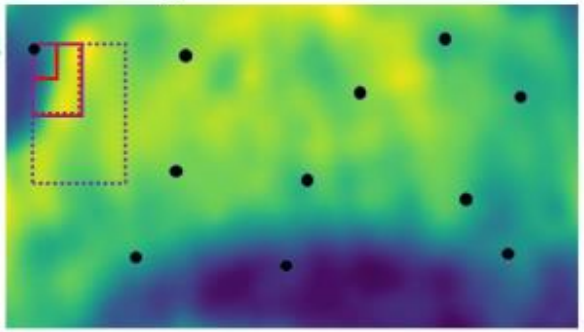
$$\varepsilon \sim N(\mathbf{0}, \mathbf{D}_\varepsilon)$$



$\tilde{g}_i$

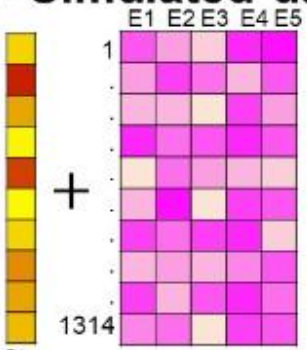
B- Real field variability trial





Uniformity trial (64 ha, 100 sites)

C- Simulated data

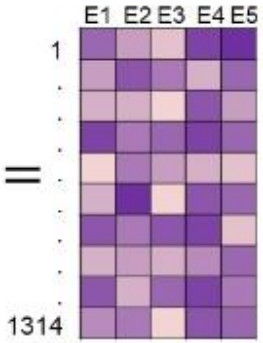


$\tilde{g}_i$ Simulated GE

Genotype by environment

GE:G (σ_{ge}^2: σ_g^2): 0.2 or 2.5

$$\mathbf{ge} \sim N(\mathbf{0}, \mathbf{K} \otimes \mathbf{I}\sigma_{ge}^2)$$



Genotypic effects (g_{ij})

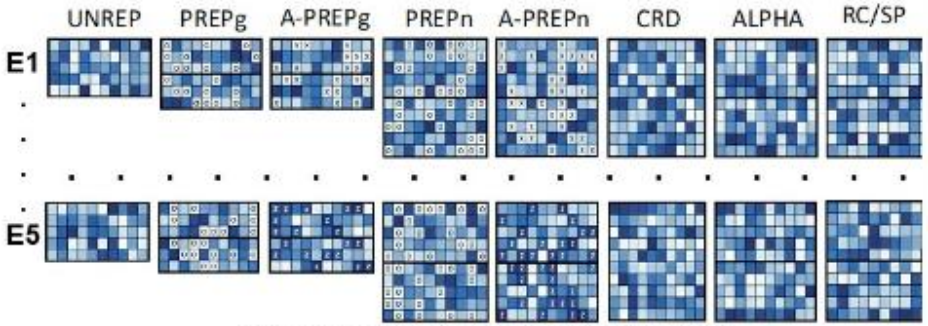
Simulated yield

$$y_{ijk}^{SIM} = g_{ij} + \varepsilon_{ijk}^{*} + \delta_{ijk}$$

$$\delta_{ijk} \sim N\left(0, 2\left(\left(\frac{1-h^2}{h^2}\right)\sigma_{g*}^2\right) - \sigma_{\varepsilon_{ijk}^{*}}^2\right)$$

Heritability h^2: 0.3 or 0.8

D- Experimental design



Experimental design randomization

E- Analysis model

$$y_{ijklm} = \mu + g_i + e_j + ge_{ij} + d_{k(j)} + s_{lm(j)} + \varepsilon_{ijklm}$$

$\tilde{g}_{ij}$

$$\varepsilon \sim N(\mathbf{0}, \mathbf{D}_\varepsilon)$$

Relationship among genotypes

G: I or K

$$\mathbf{g} \sim N(\mathbf{0}, \mathbf{G}\sigma_g^2)$$

$$\mathbf{ge} \sim N(\mathbf{0}, \mathbf{G} \otimes \mathbf{I}\sigma_{ge}^2)$$

Spatial corrections

NSC $s_{lm(j)} = \emptyset$

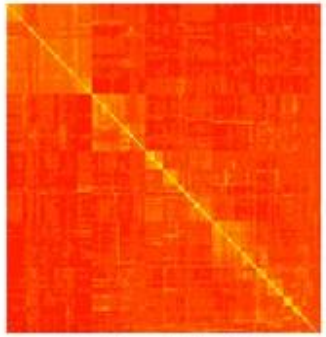
AR1xAR1 $s_{lm(j)} = r_{l(j)} + c_{m(j)}$

$$\mathbf{r} \sim N(\mathbf{0}, \mathbf{D}_R \otimes \mathbf{AR1})$$

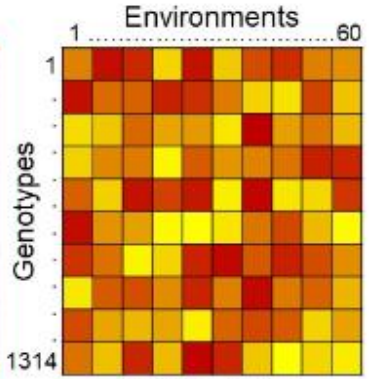
$$\mathbf{c} \sim N(\mathbf{0}, \mathbf{D}_C \otimes \mathbf{AR1})$$

A- Real wheat data

Phenotypic data



Marker data (K)



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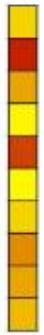

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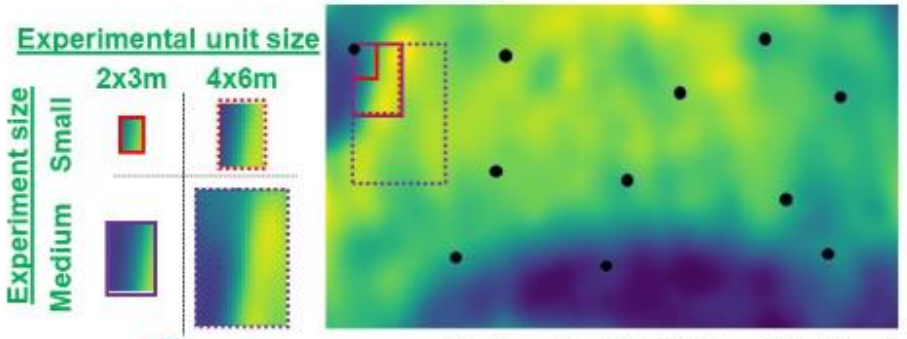

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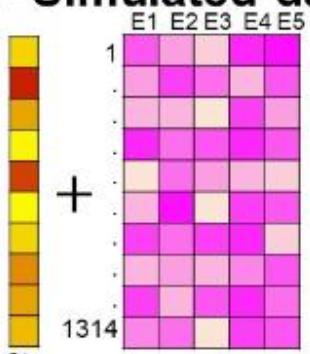

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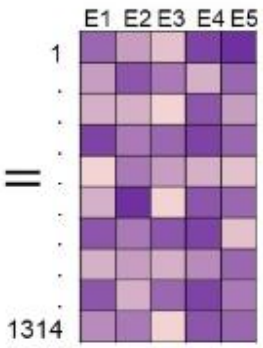

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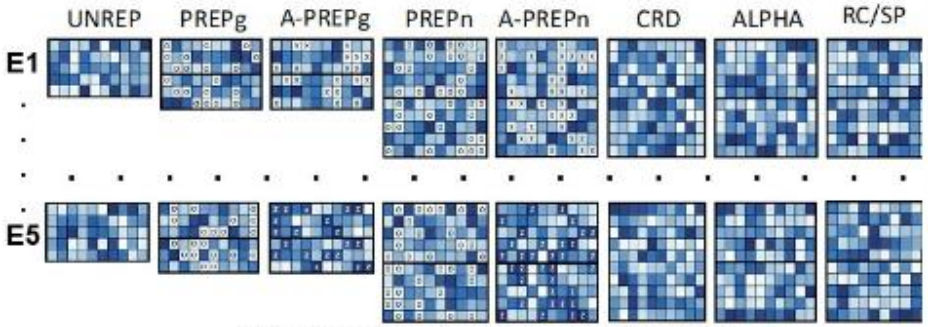

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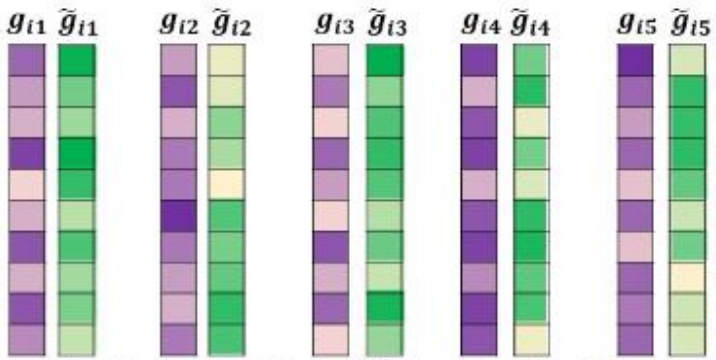

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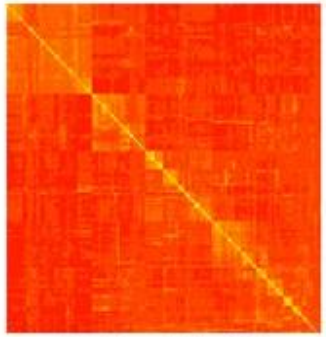

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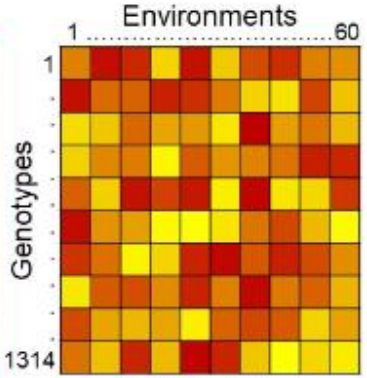

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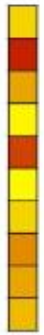

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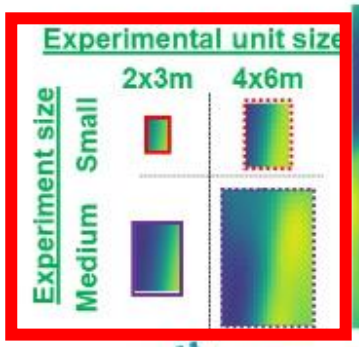

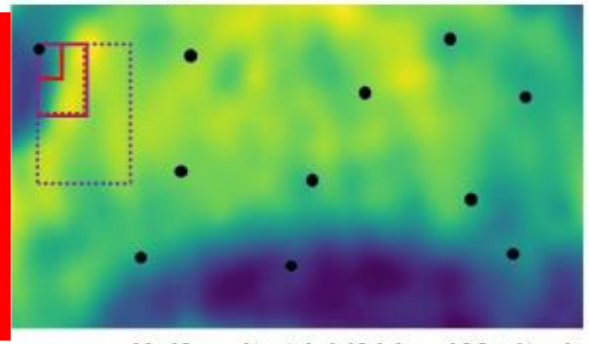

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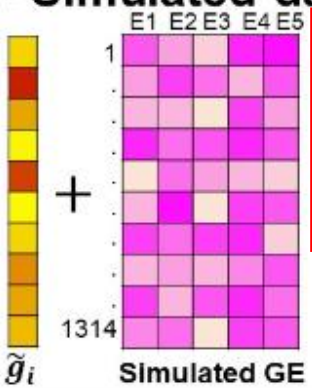

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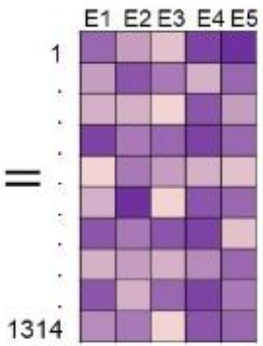

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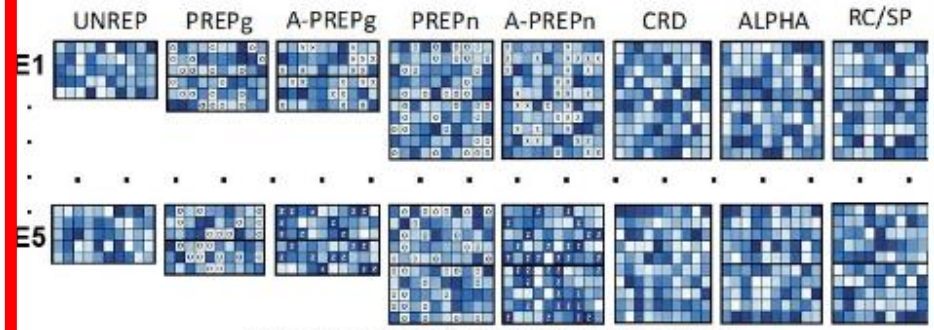

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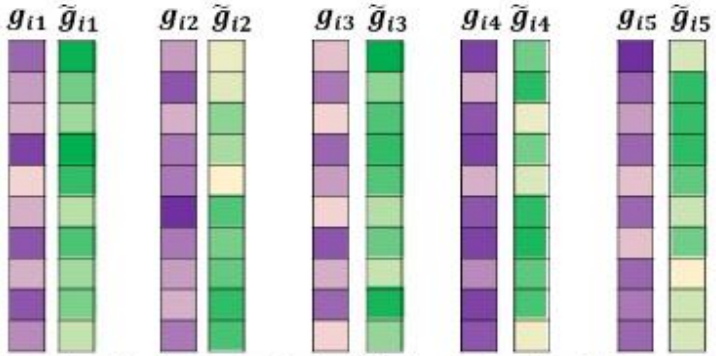

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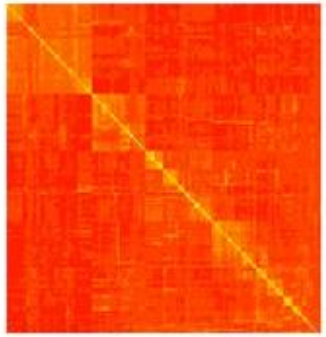

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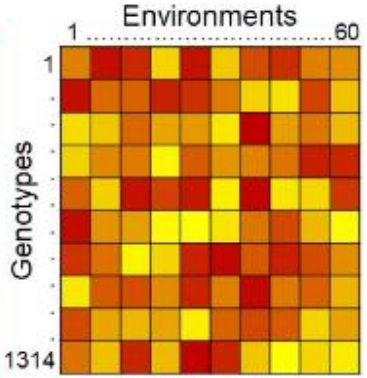

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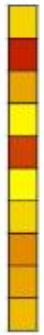

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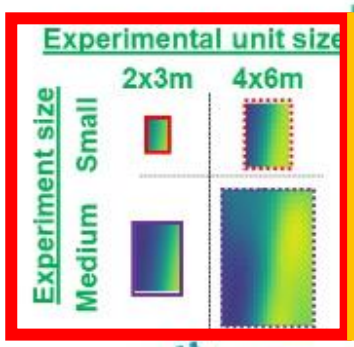

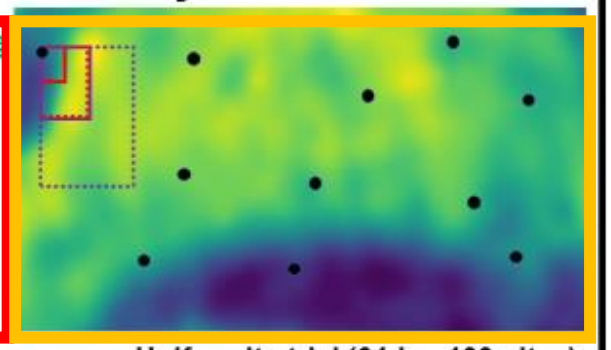

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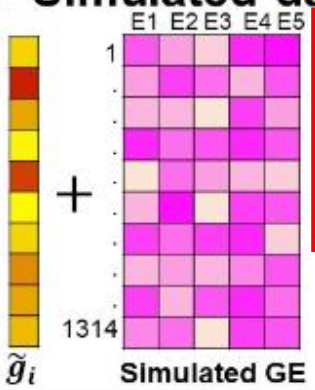

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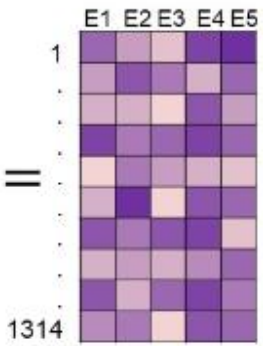

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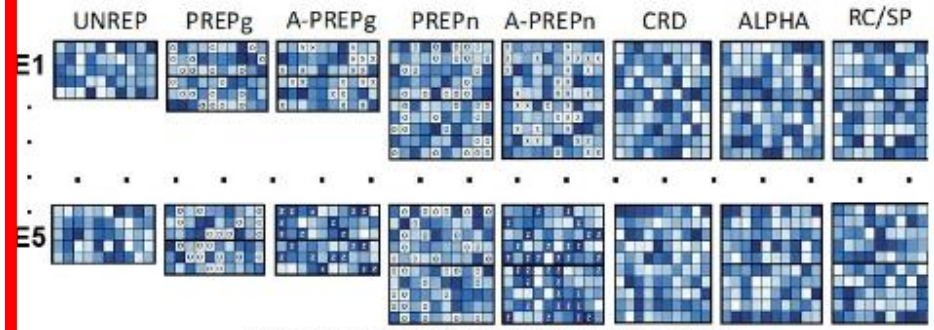

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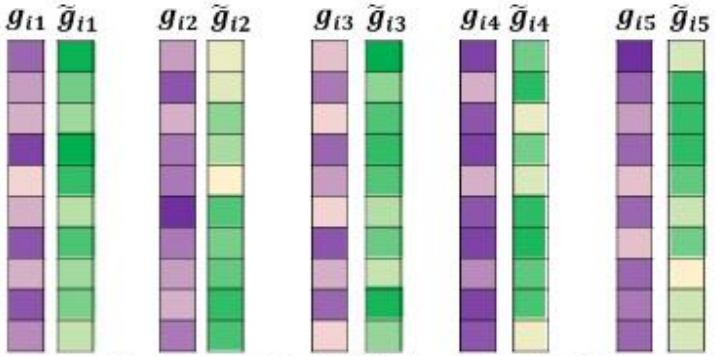

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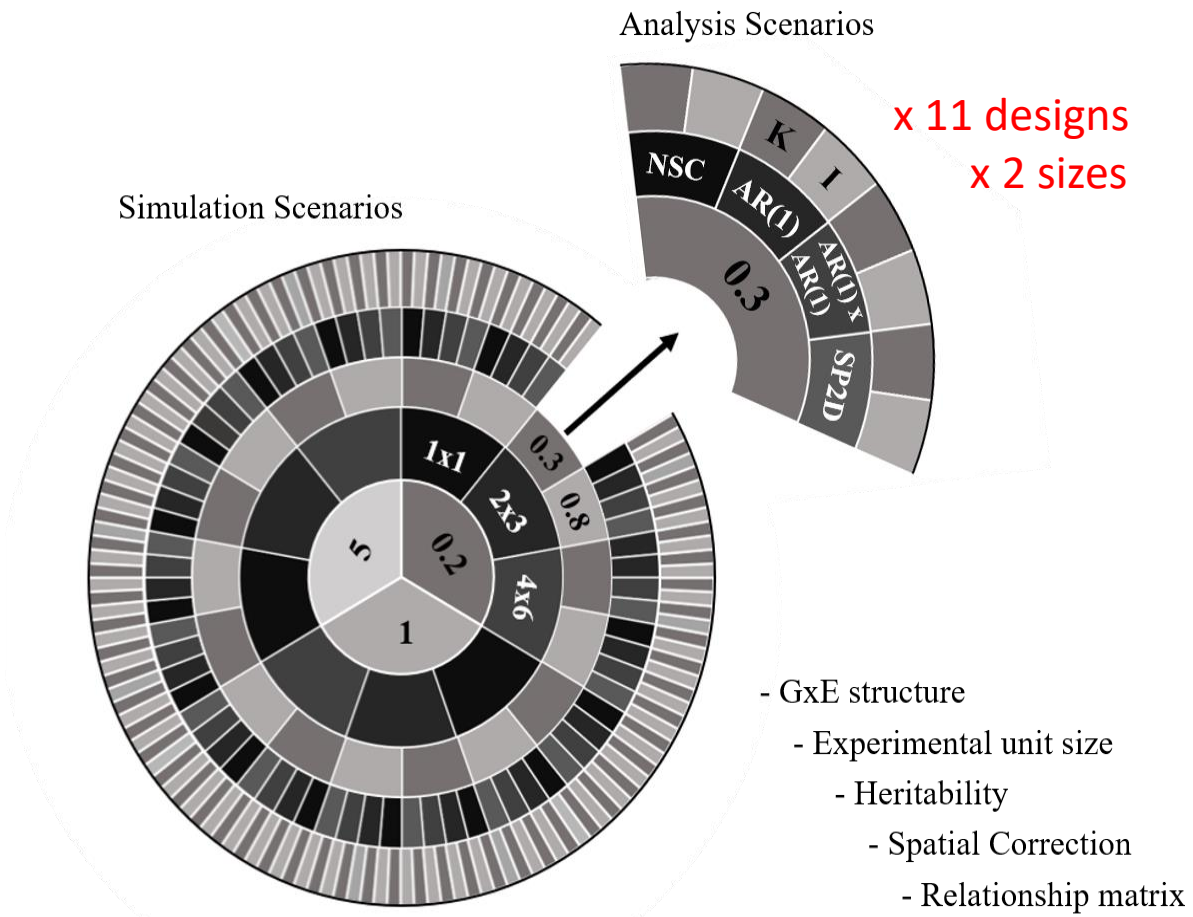

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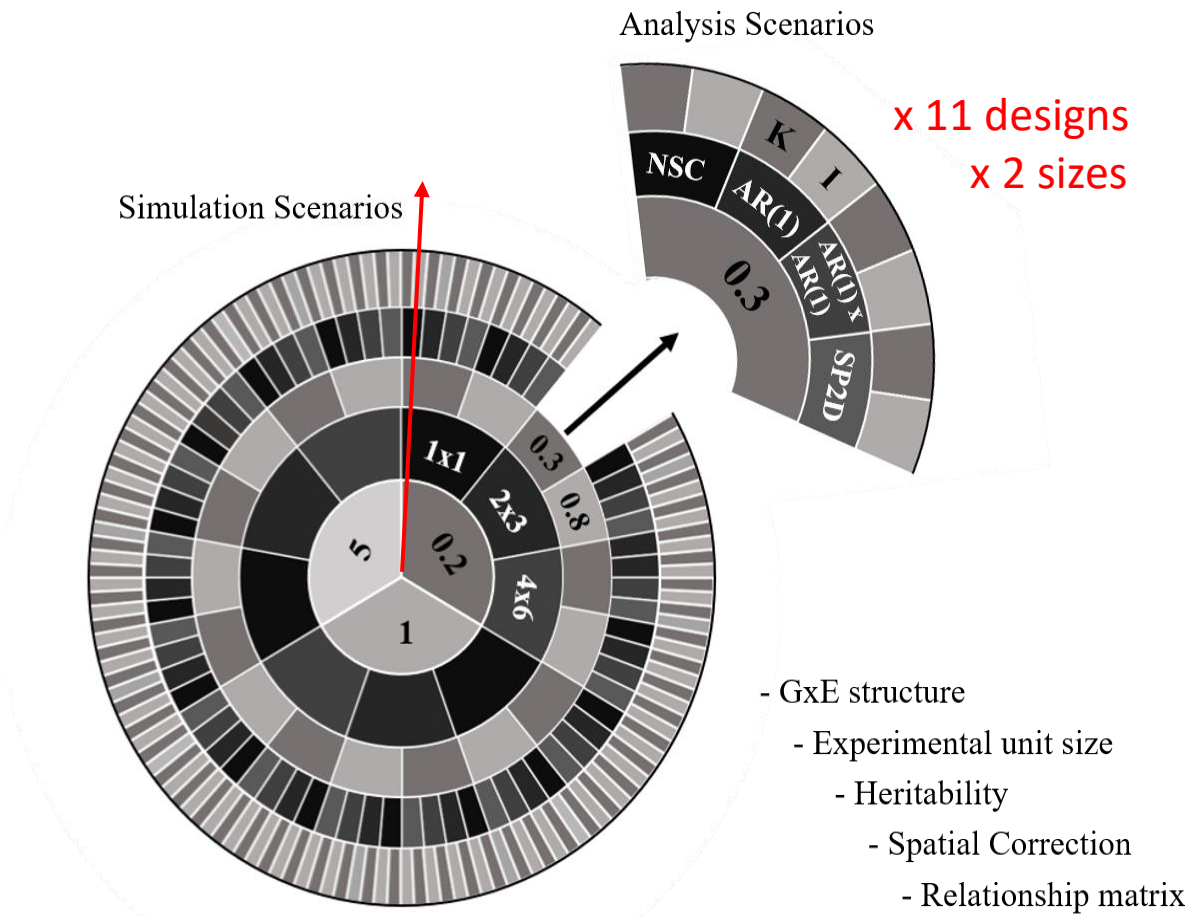

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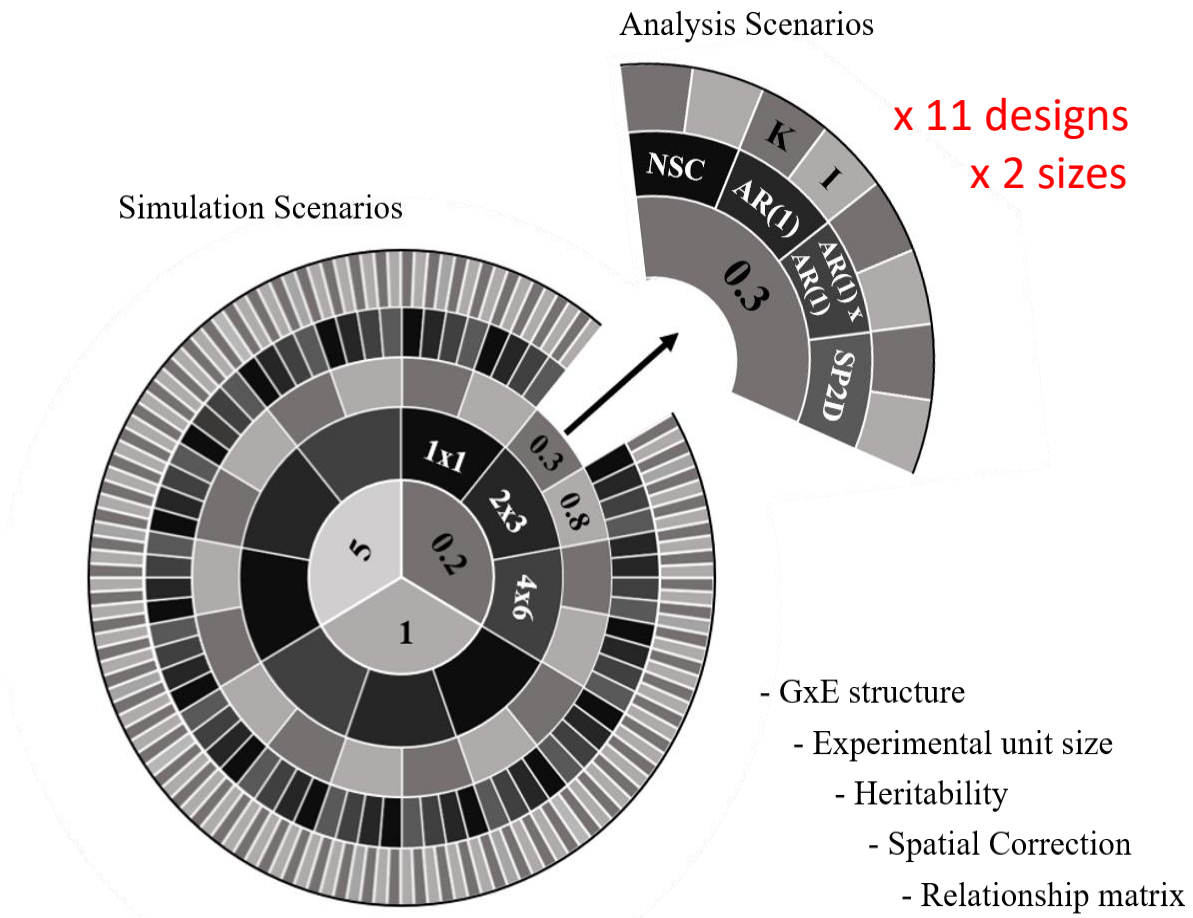

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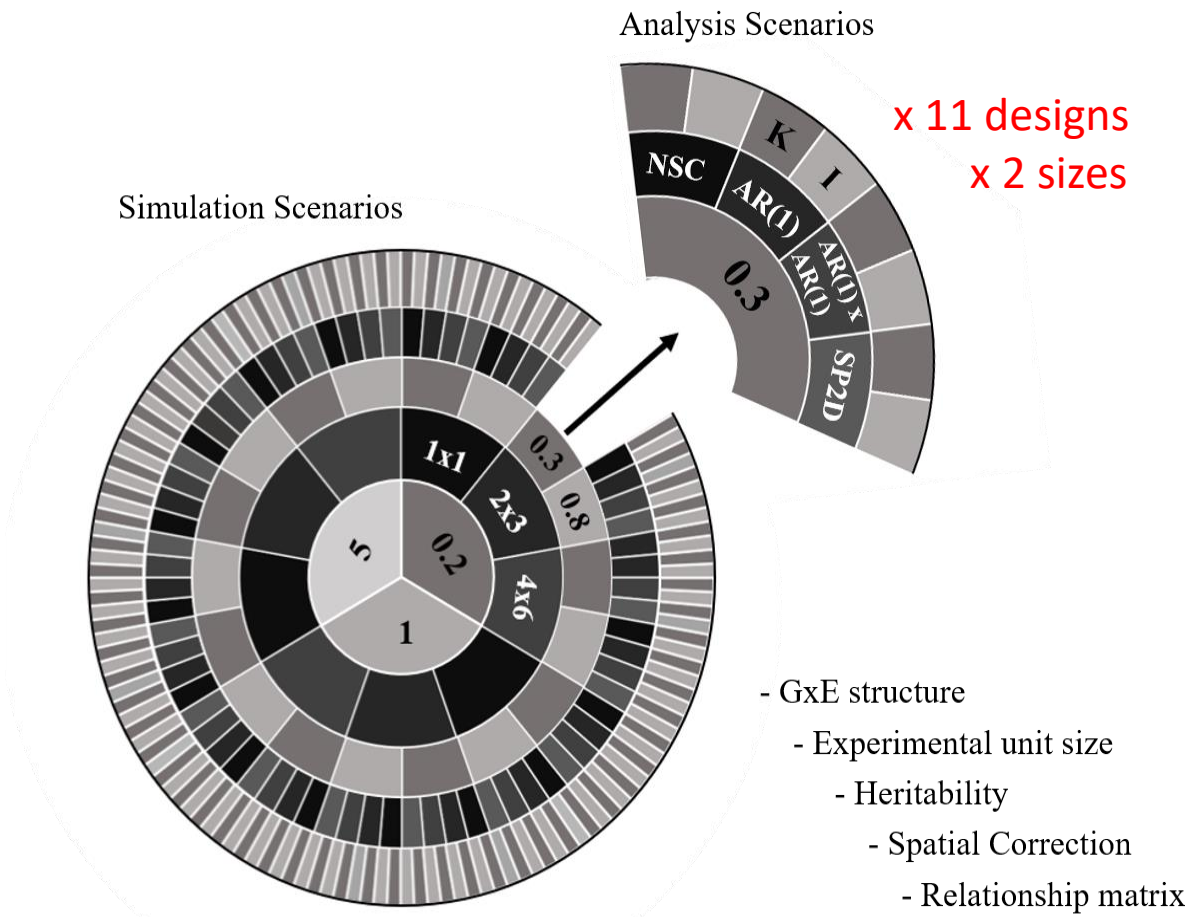

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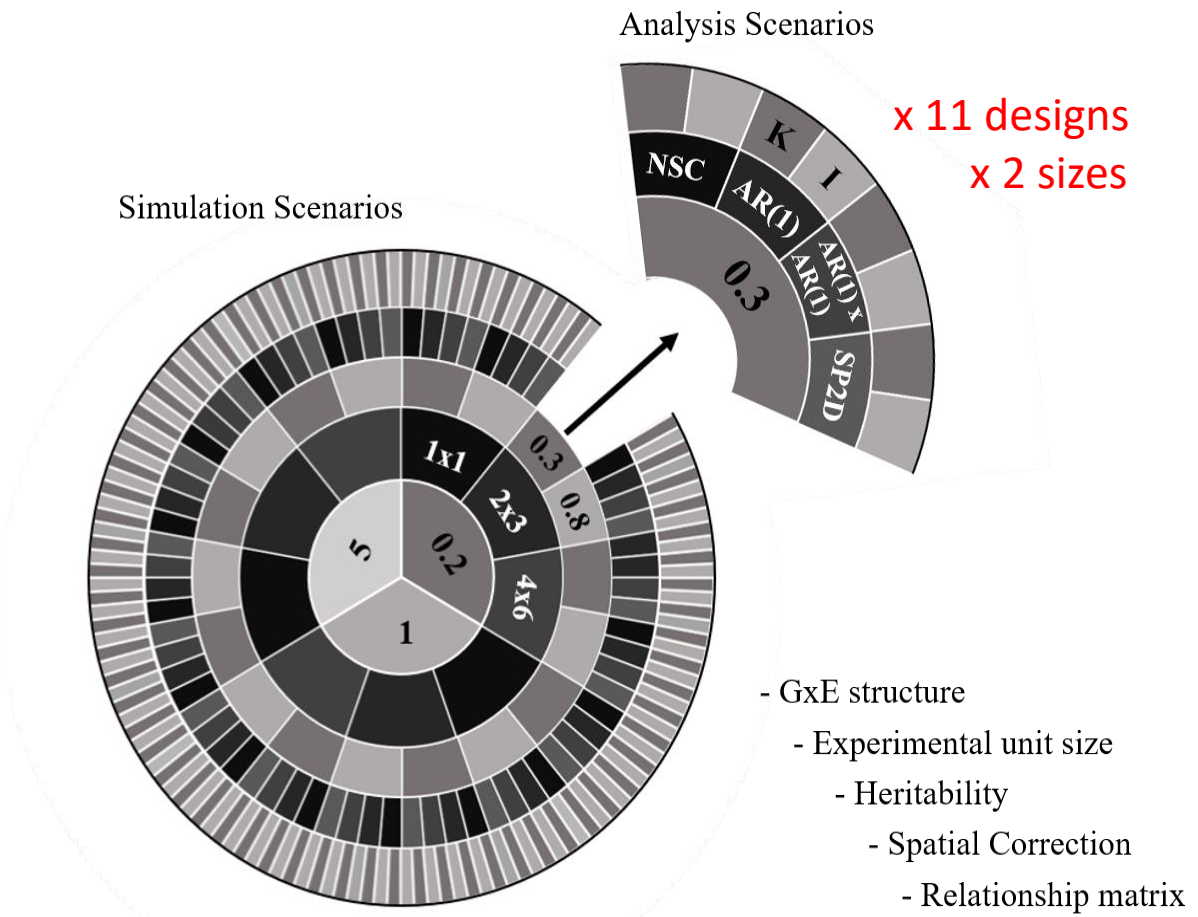

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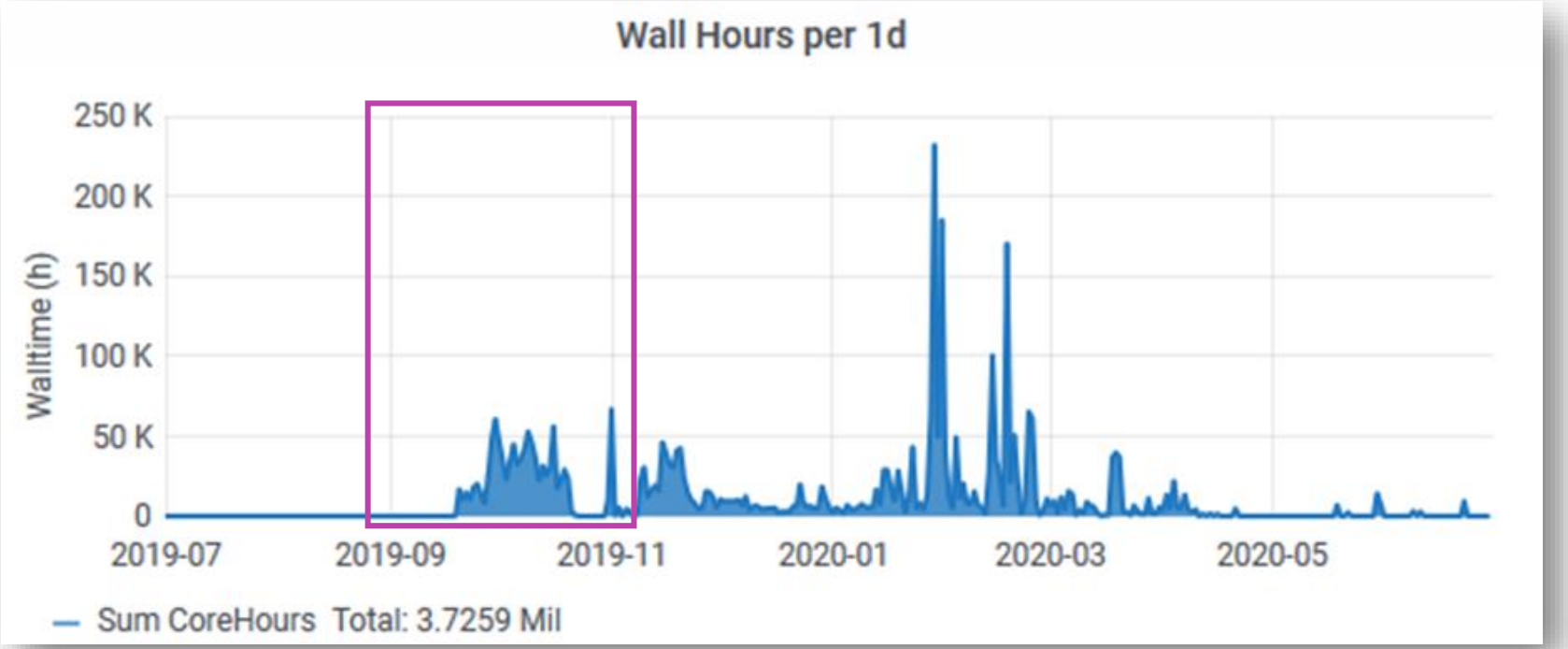

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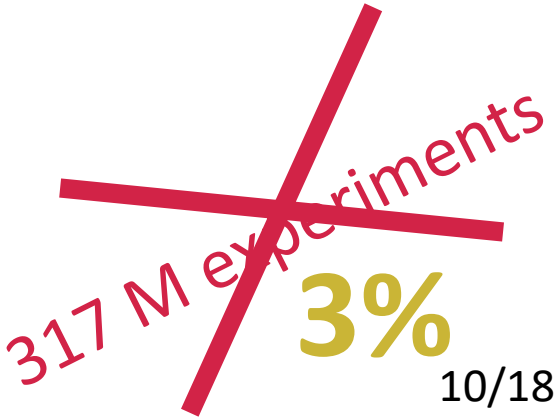

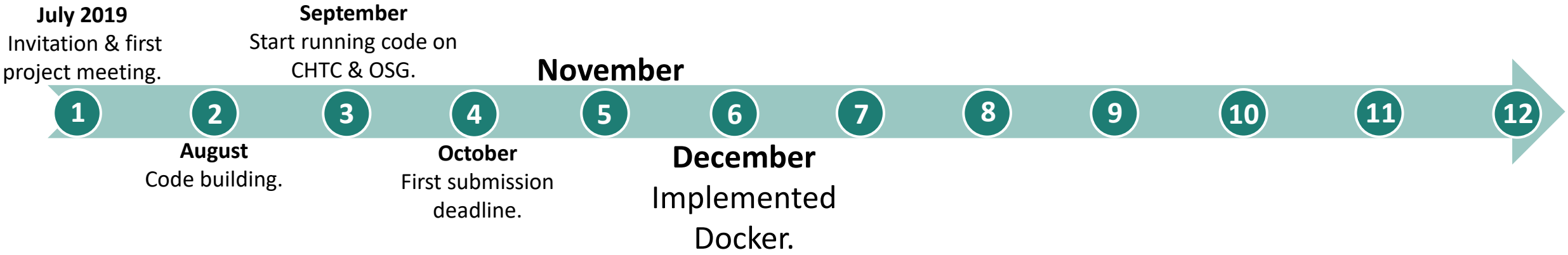
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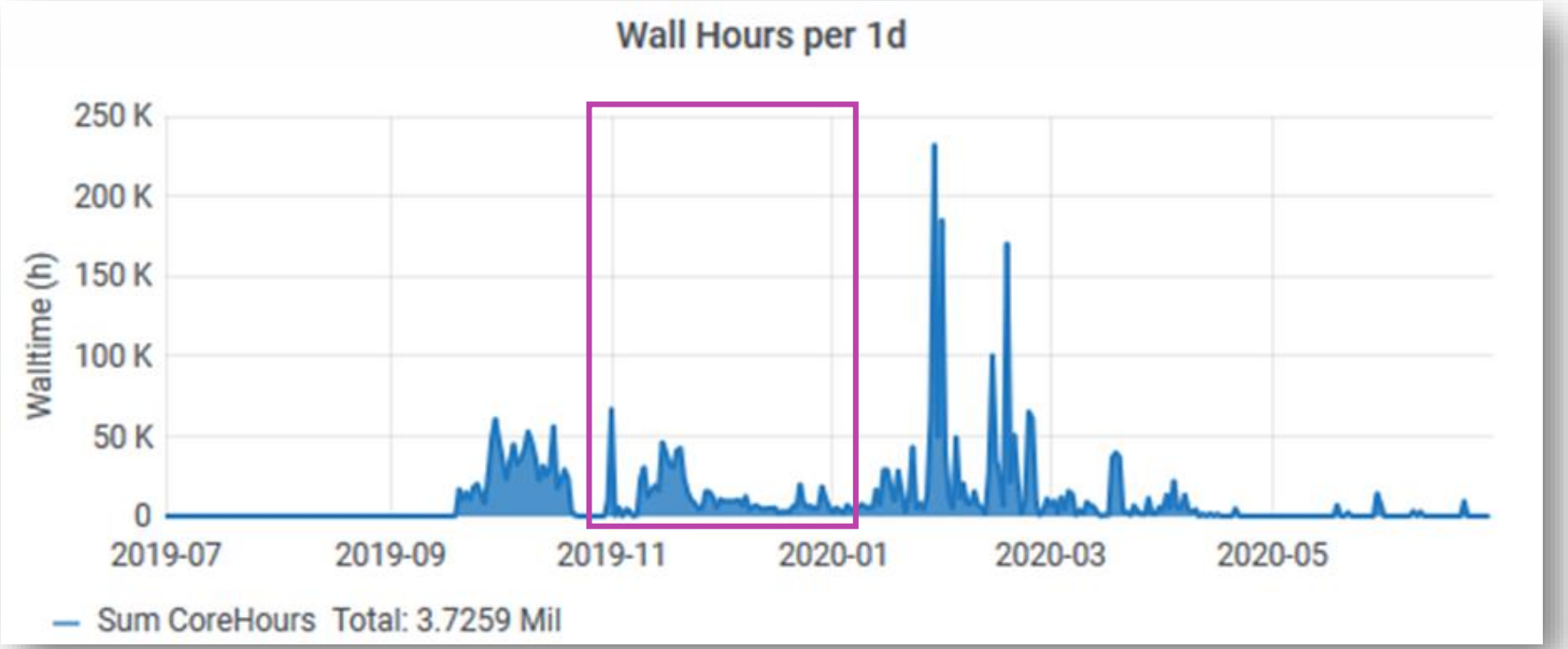

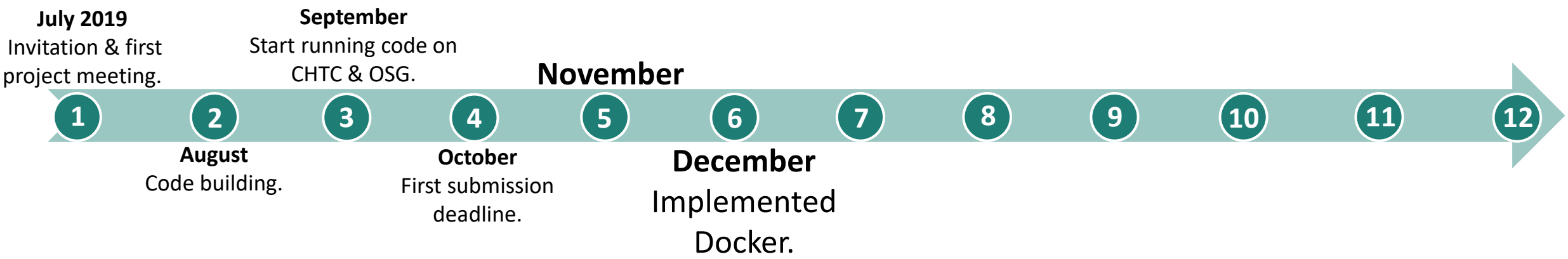

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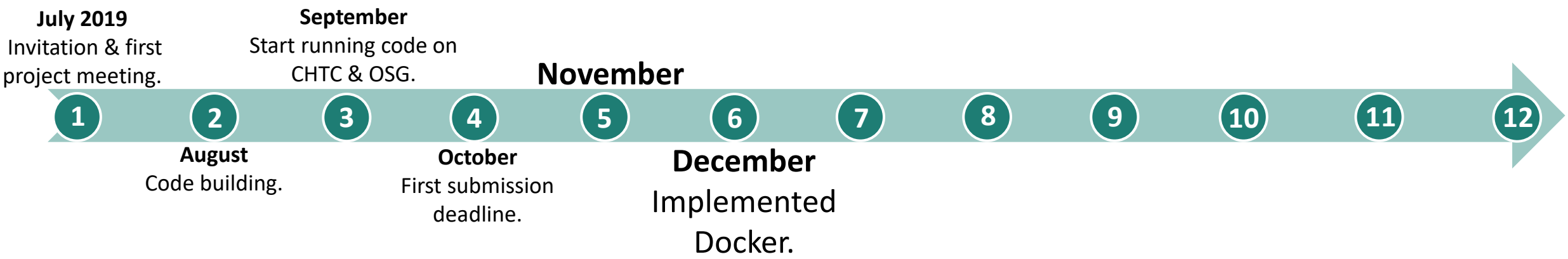

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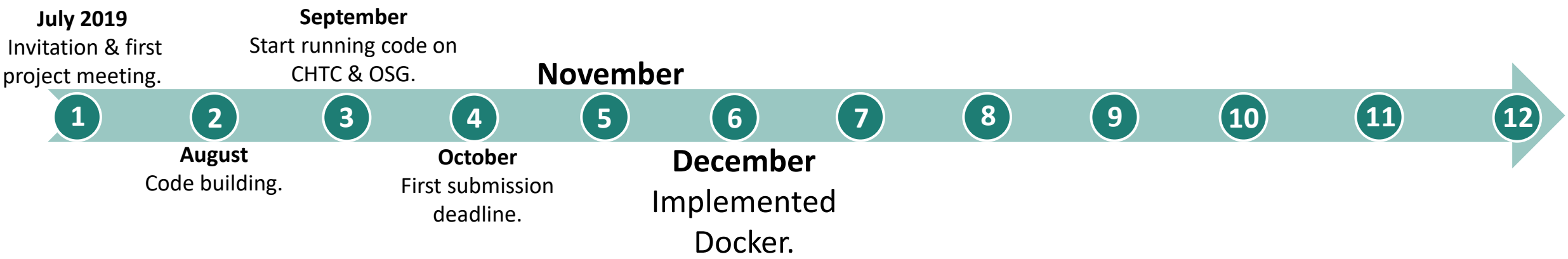

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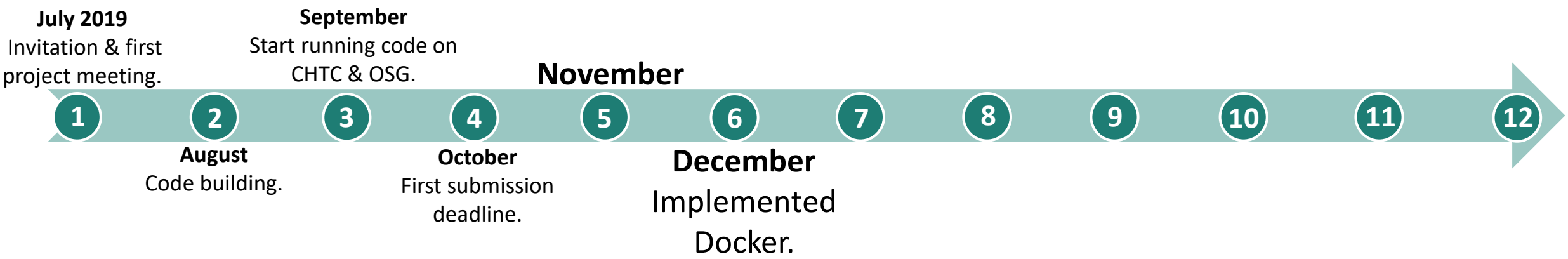

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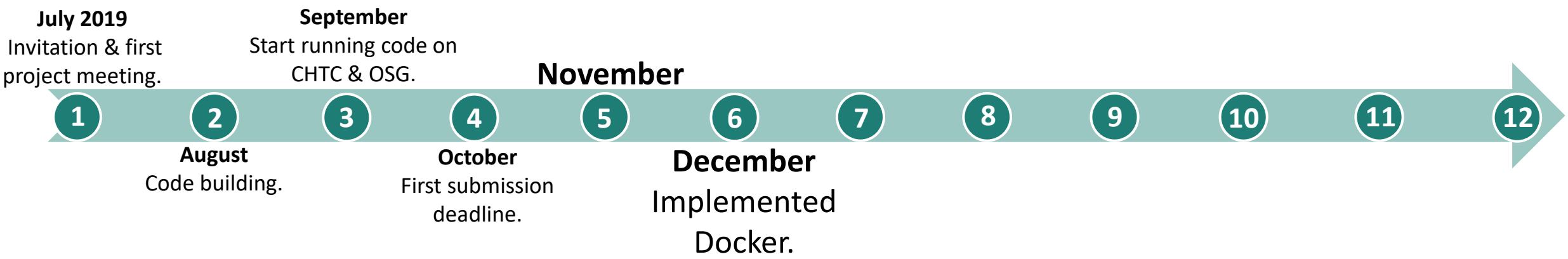

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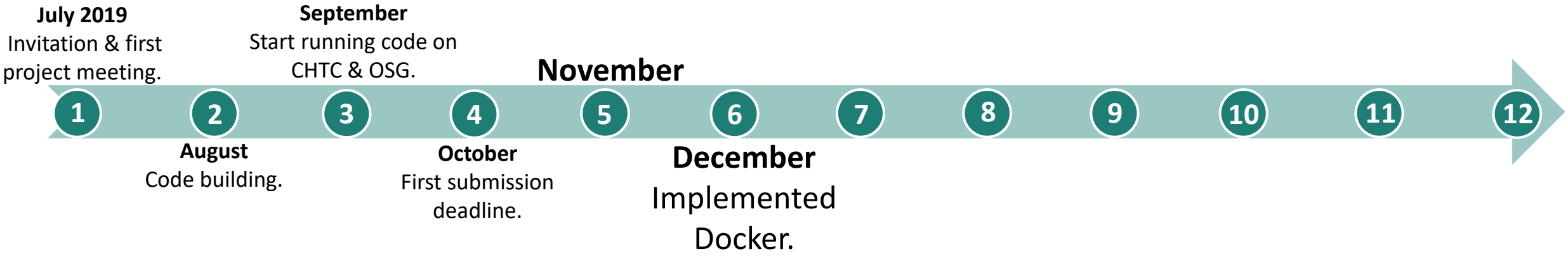

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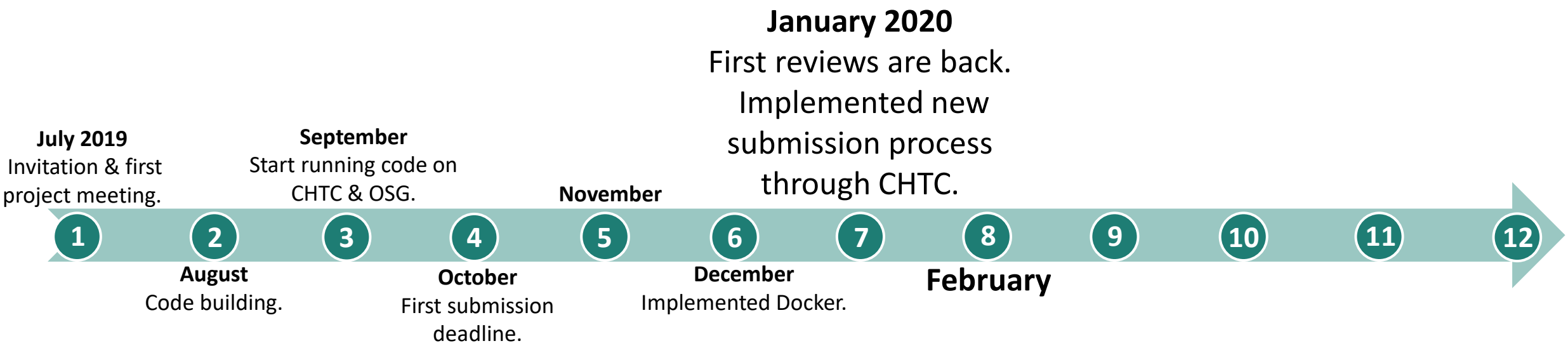
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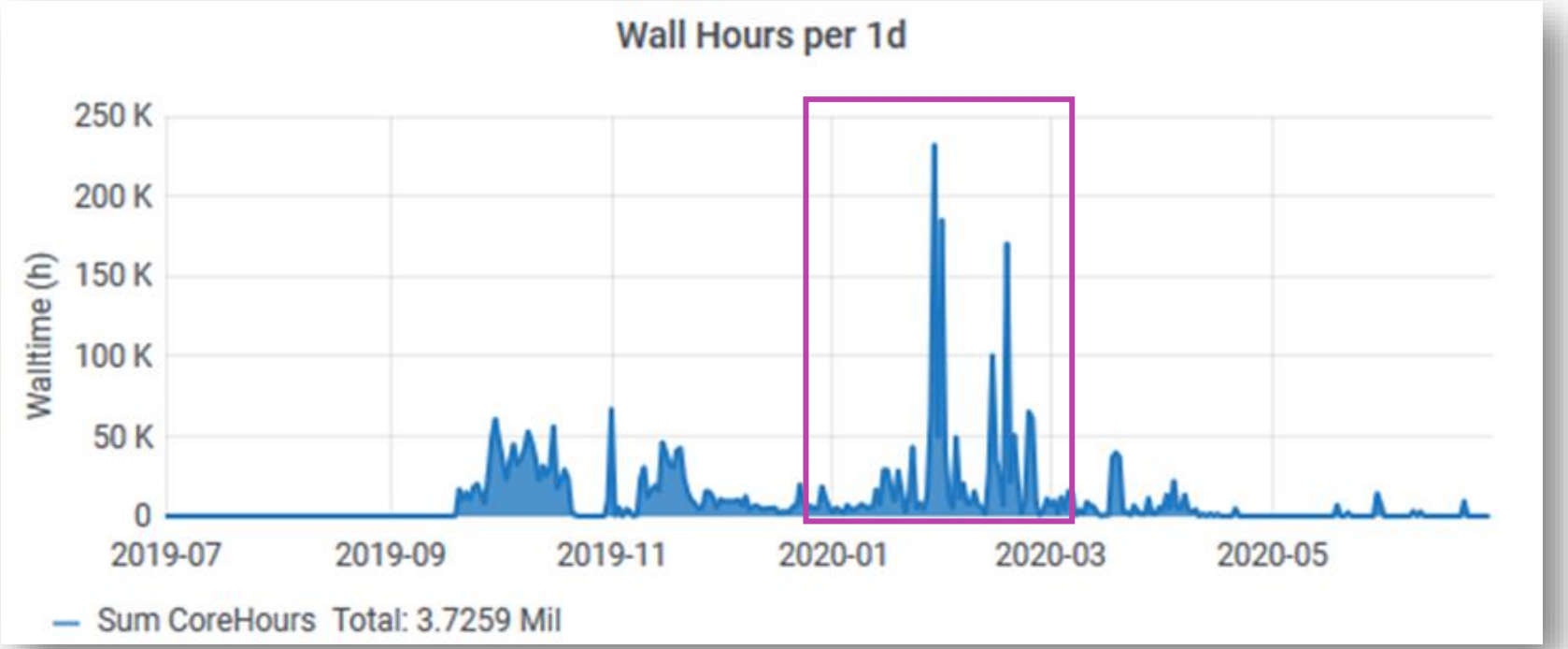

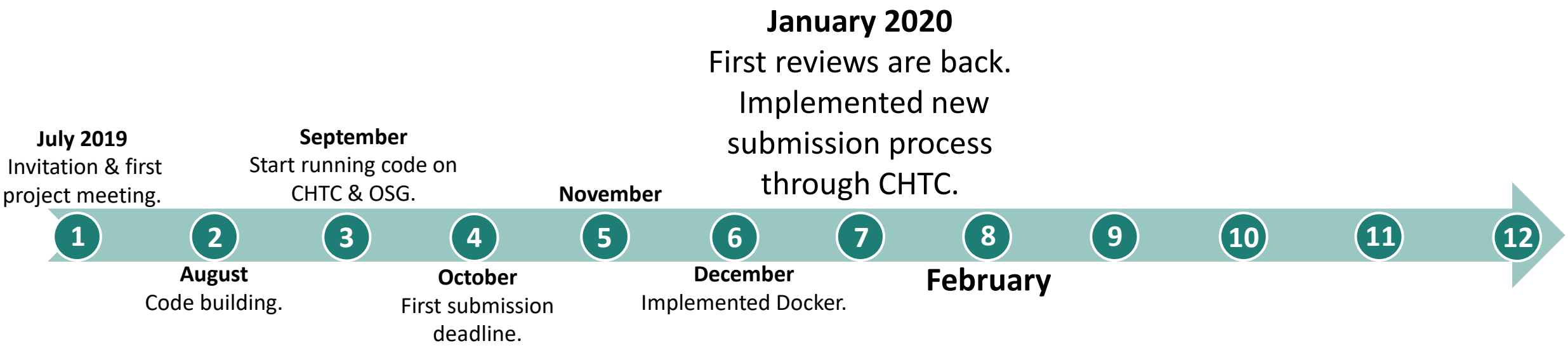

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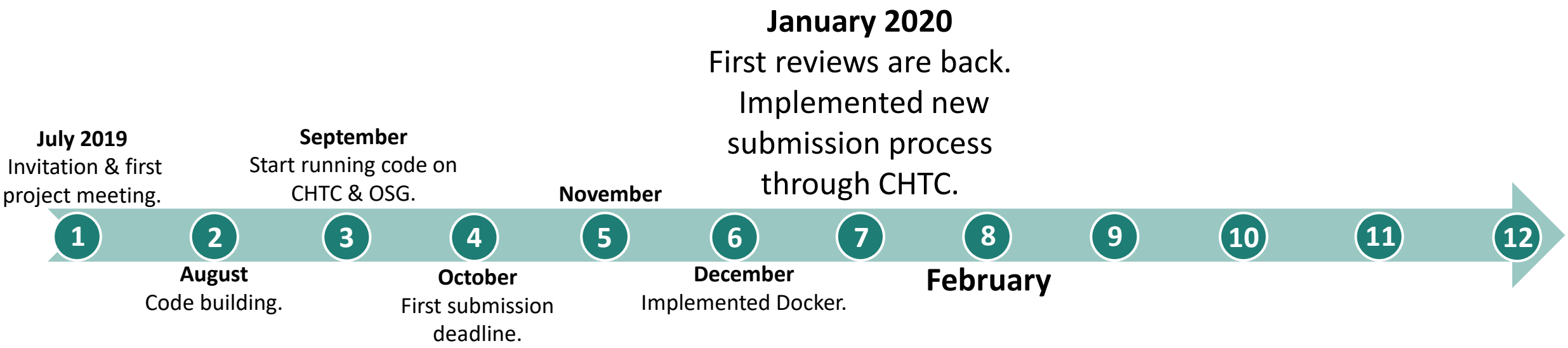

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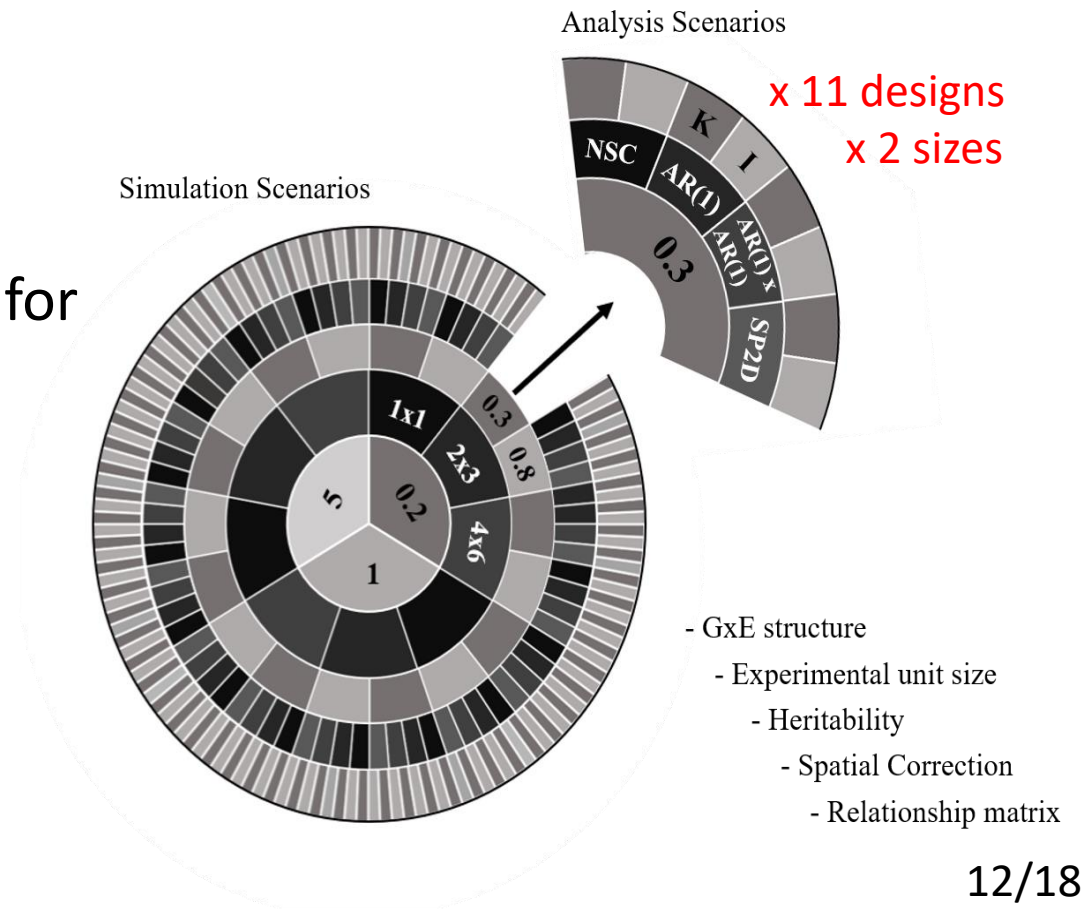

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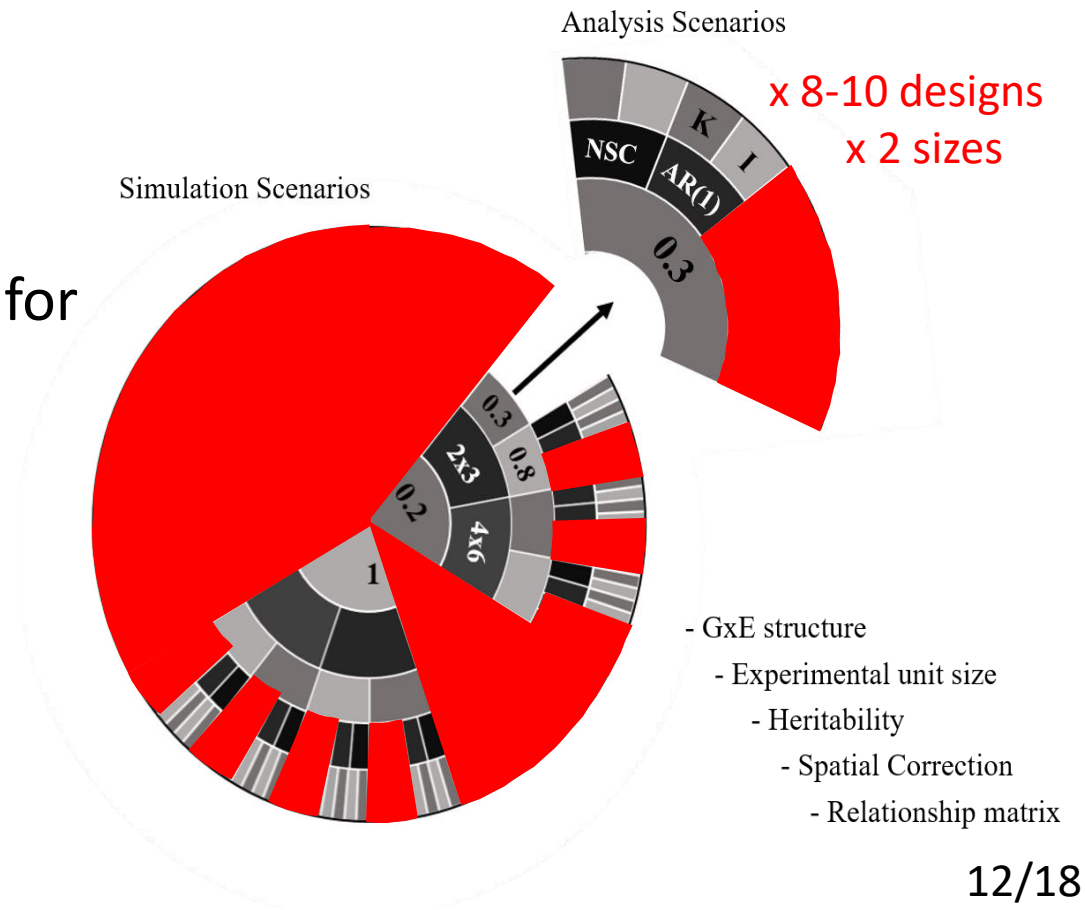

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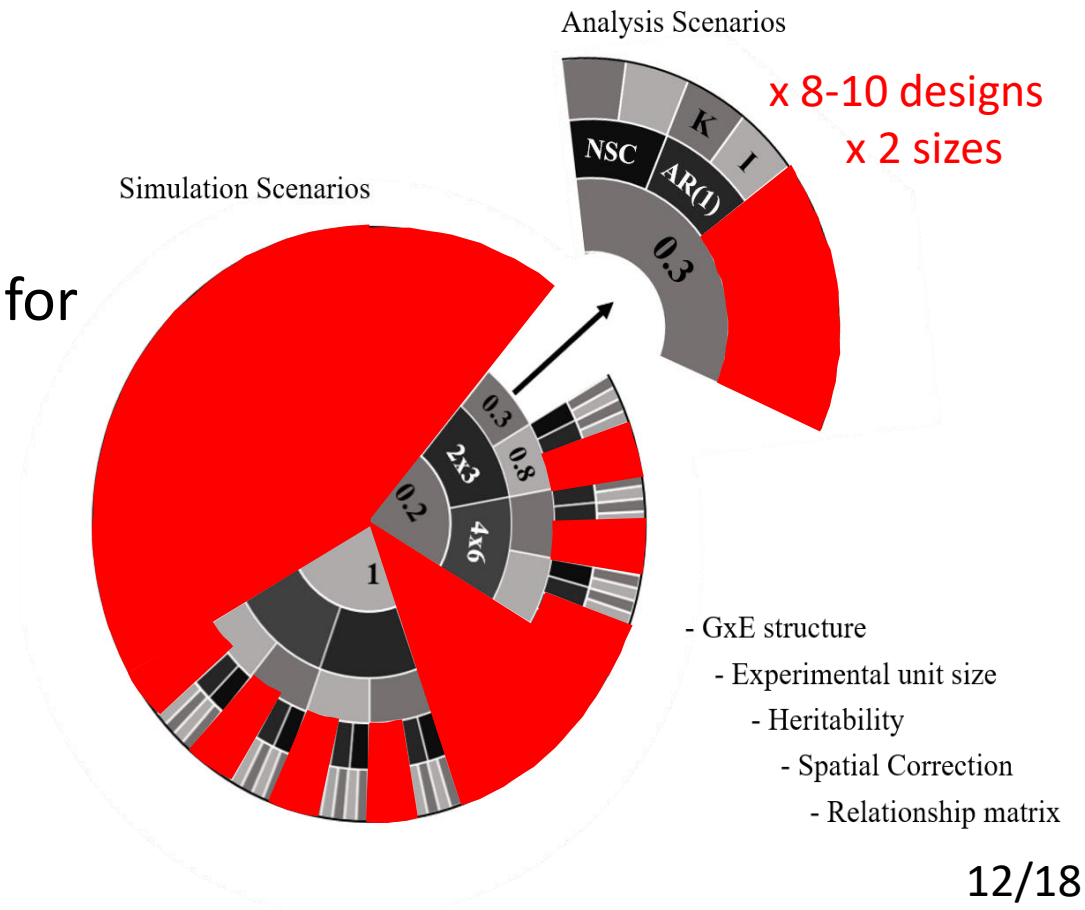

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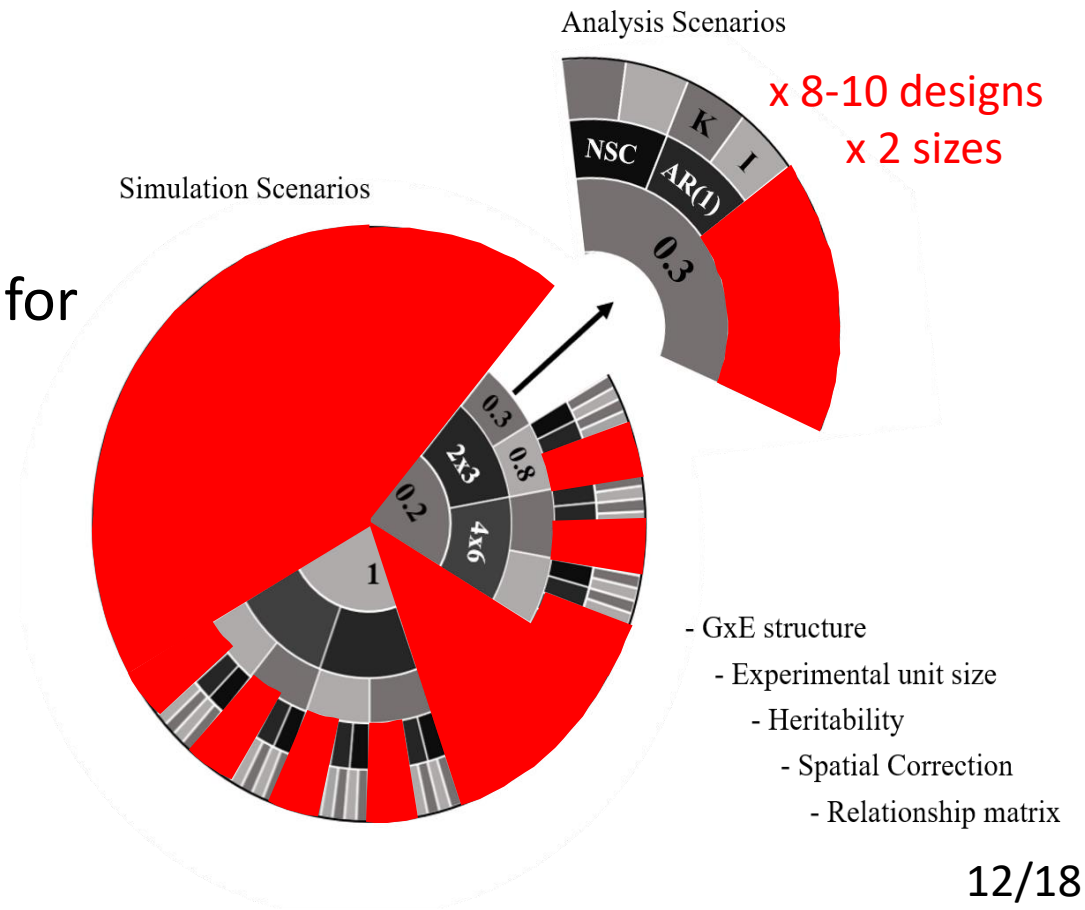
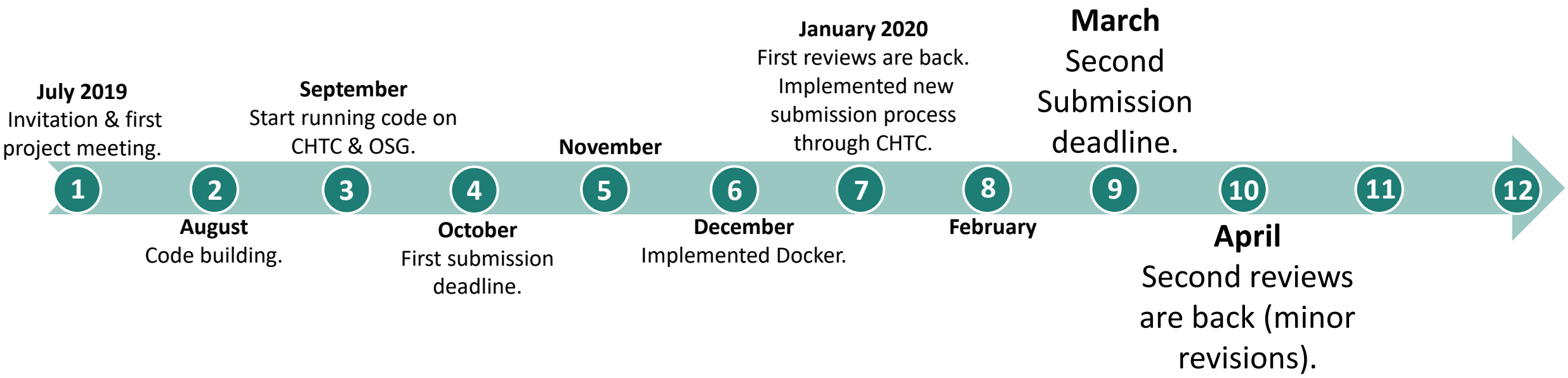
  - Old method: 3 files created for every job submitted.
  - New method: 3 files total.

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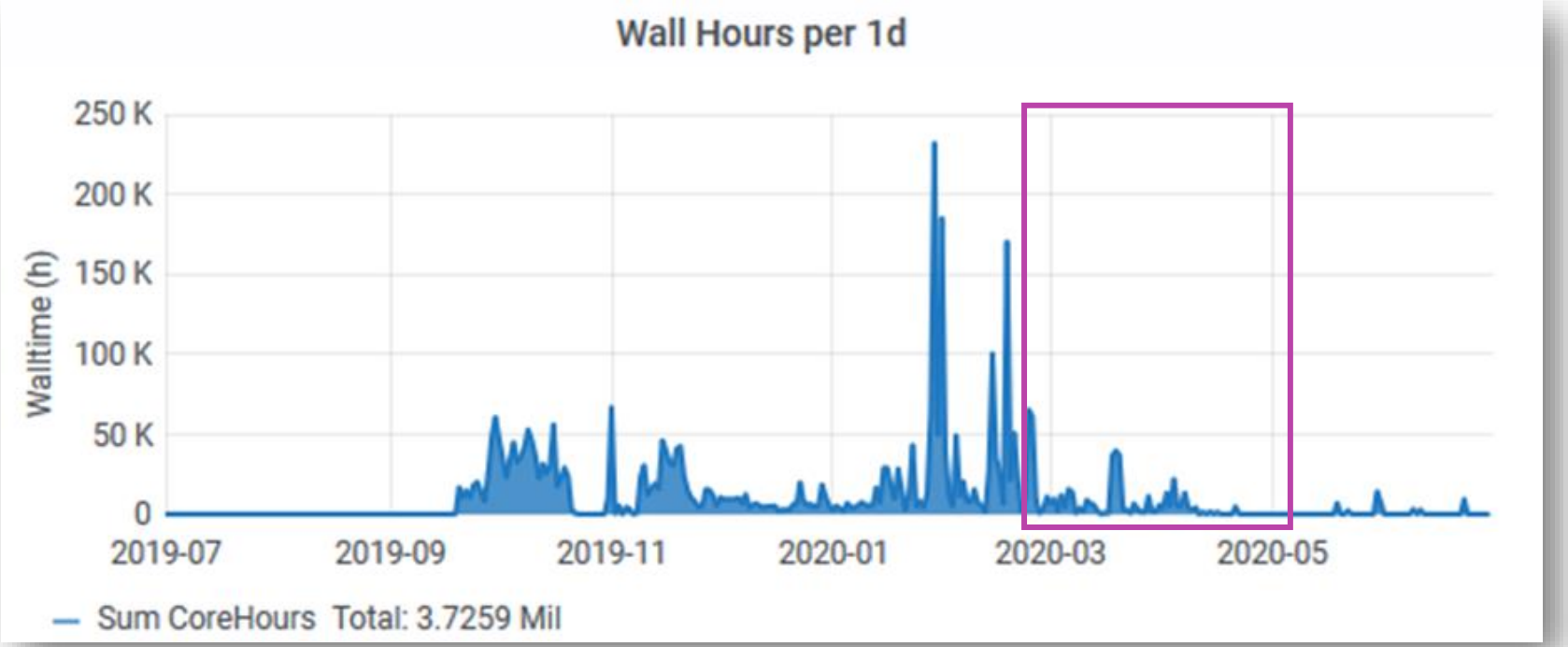

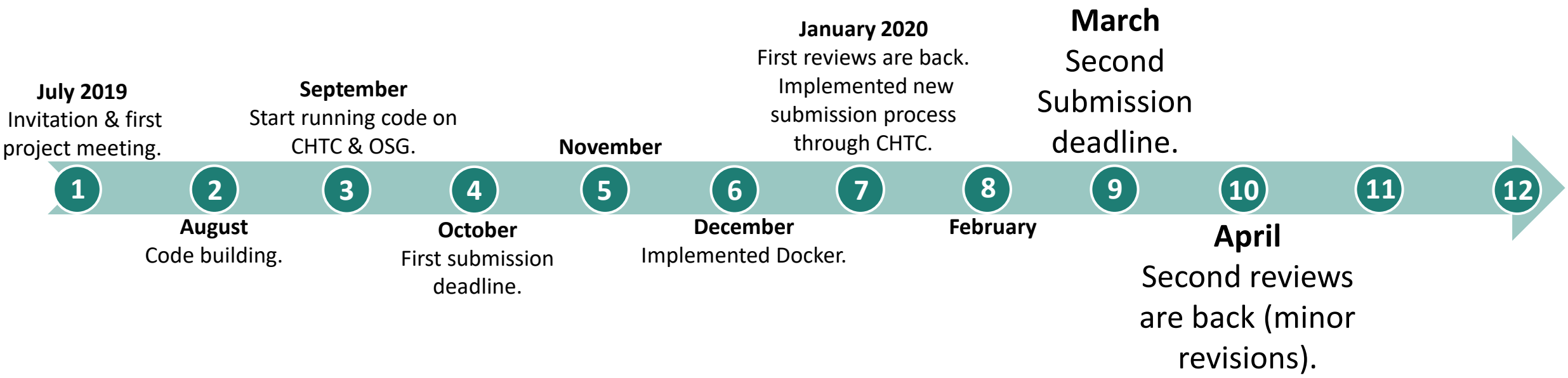

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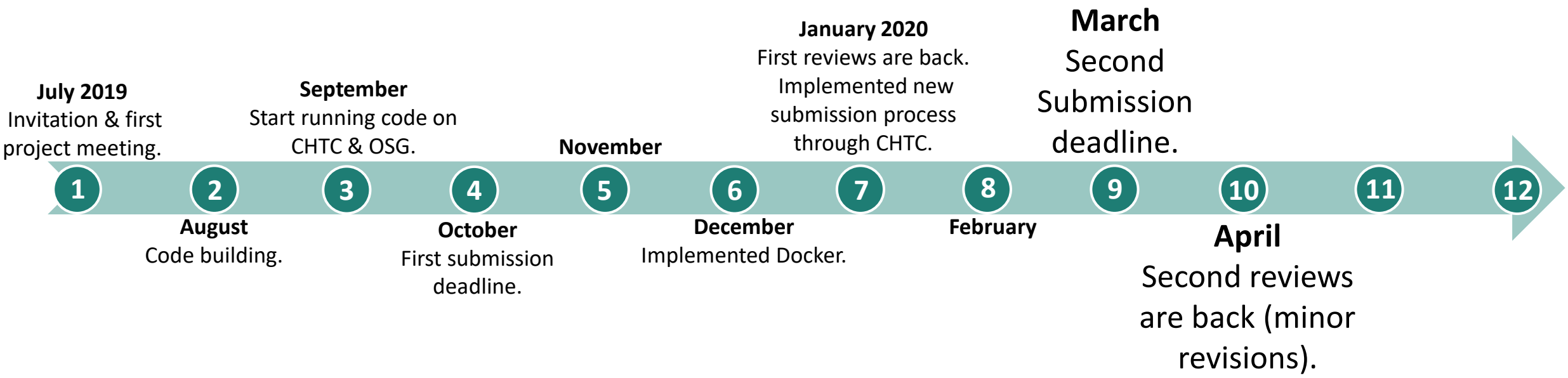

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- Better estimates of timing.

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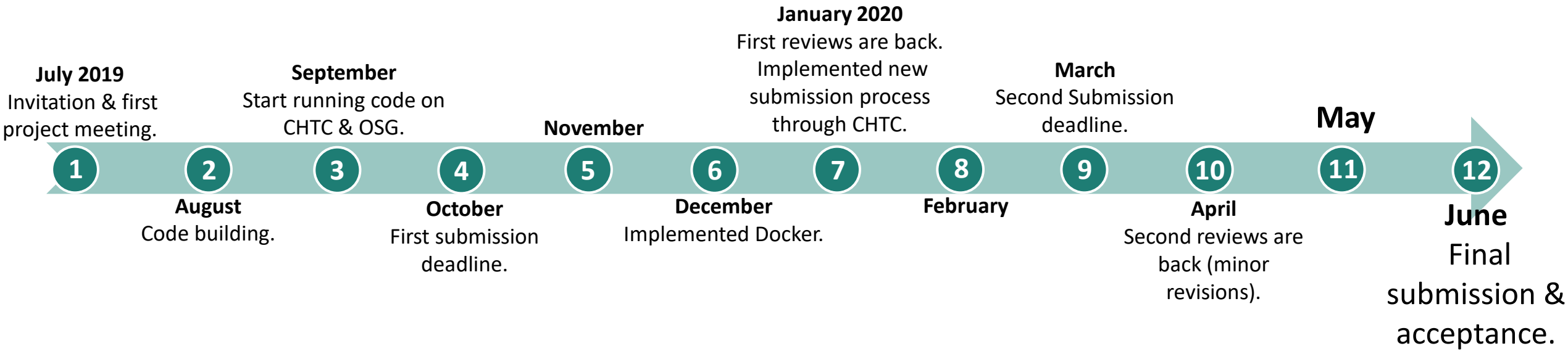
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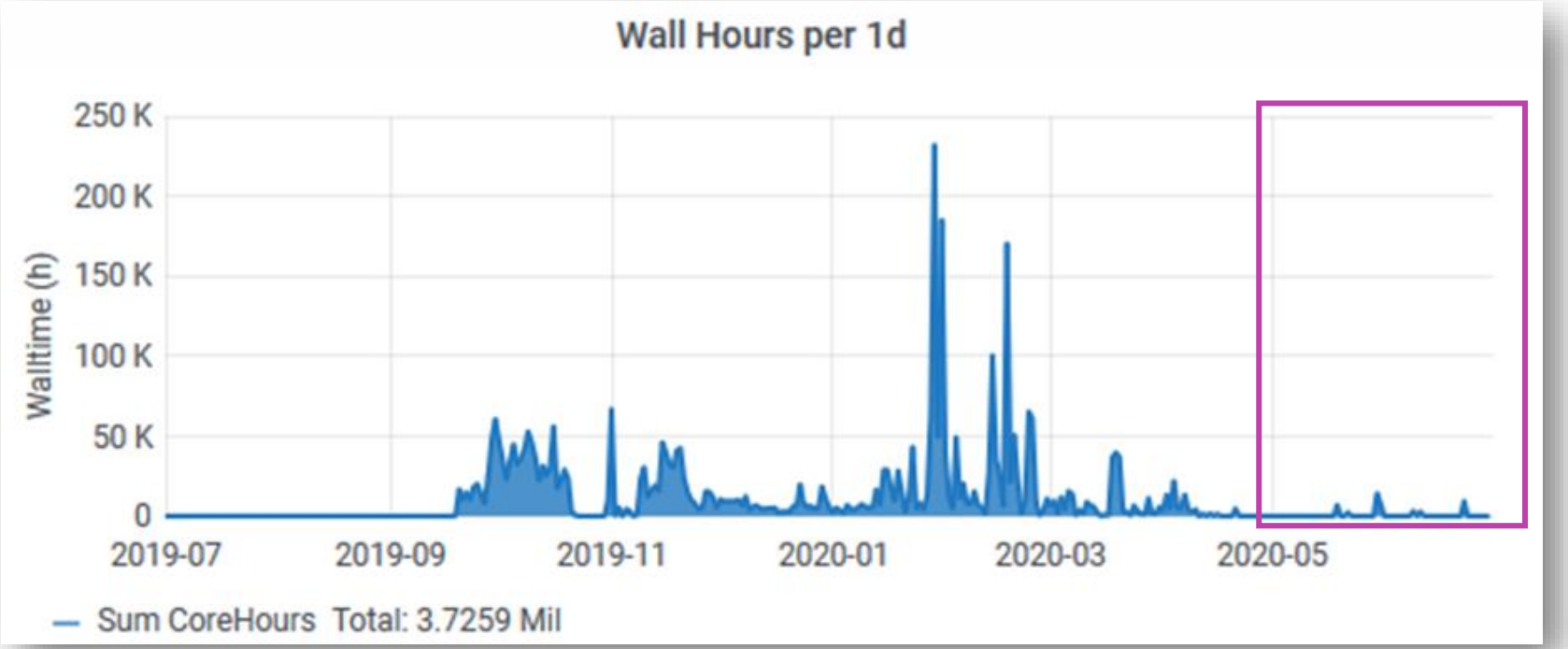

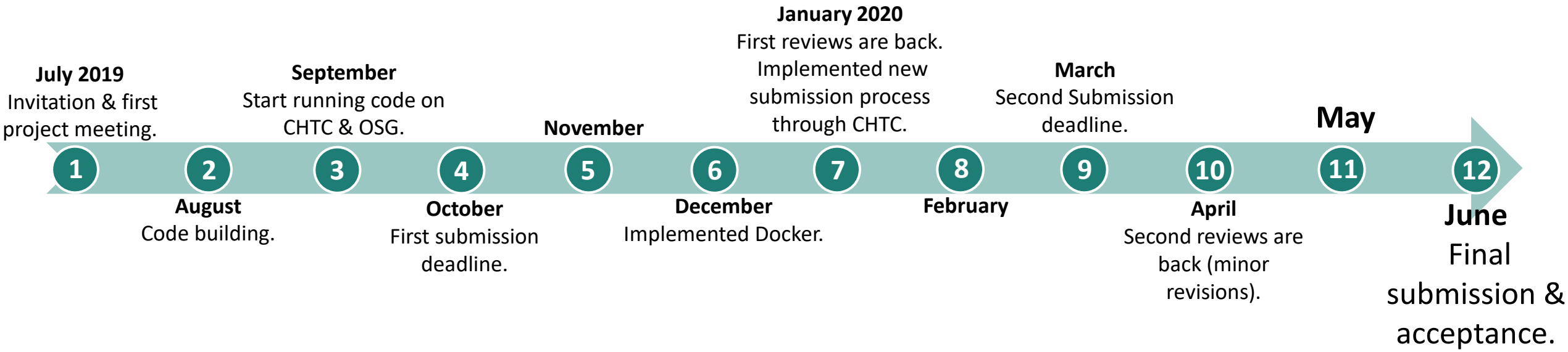

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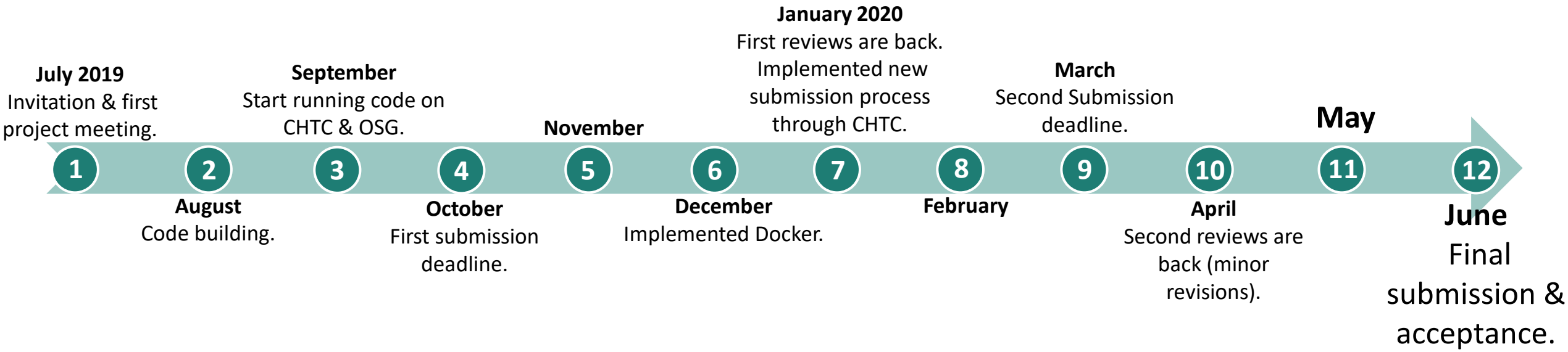

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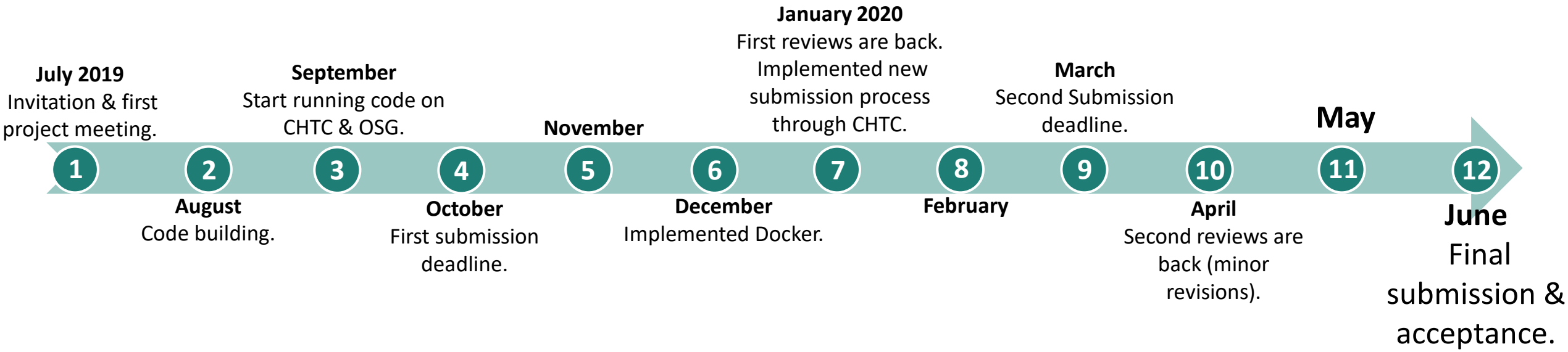

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- <u>Results</u>: ALPHA and RC designs are often better than spatial designs, and spatial corrections are more effective in larger experiments.

"Breeder's Equation"

$$R = i\underbrace{r_{g,\hat{g}}}_{\text{Correlation}}\sigma_g$$

True (g)

Predicted ($\hat{g}$)

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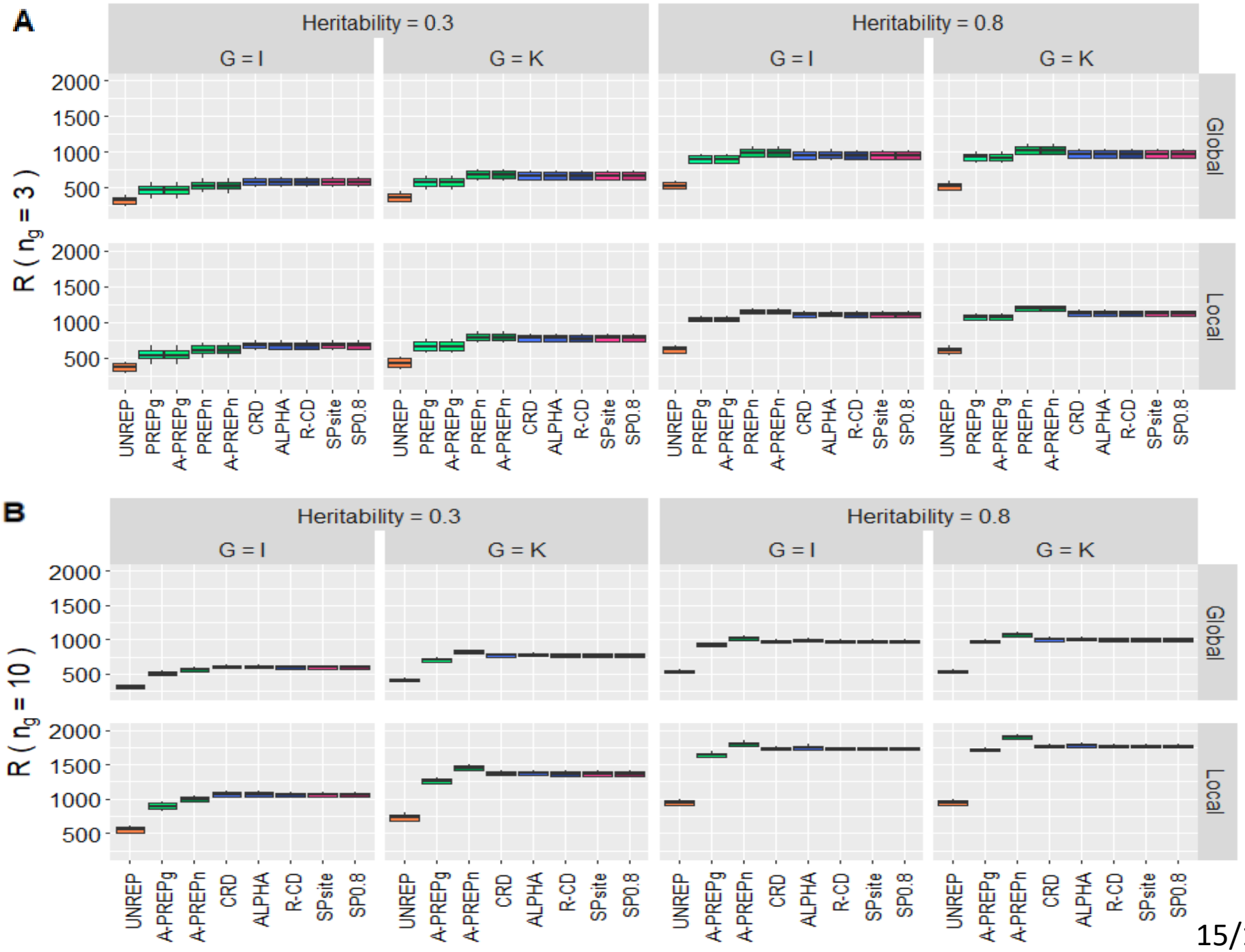

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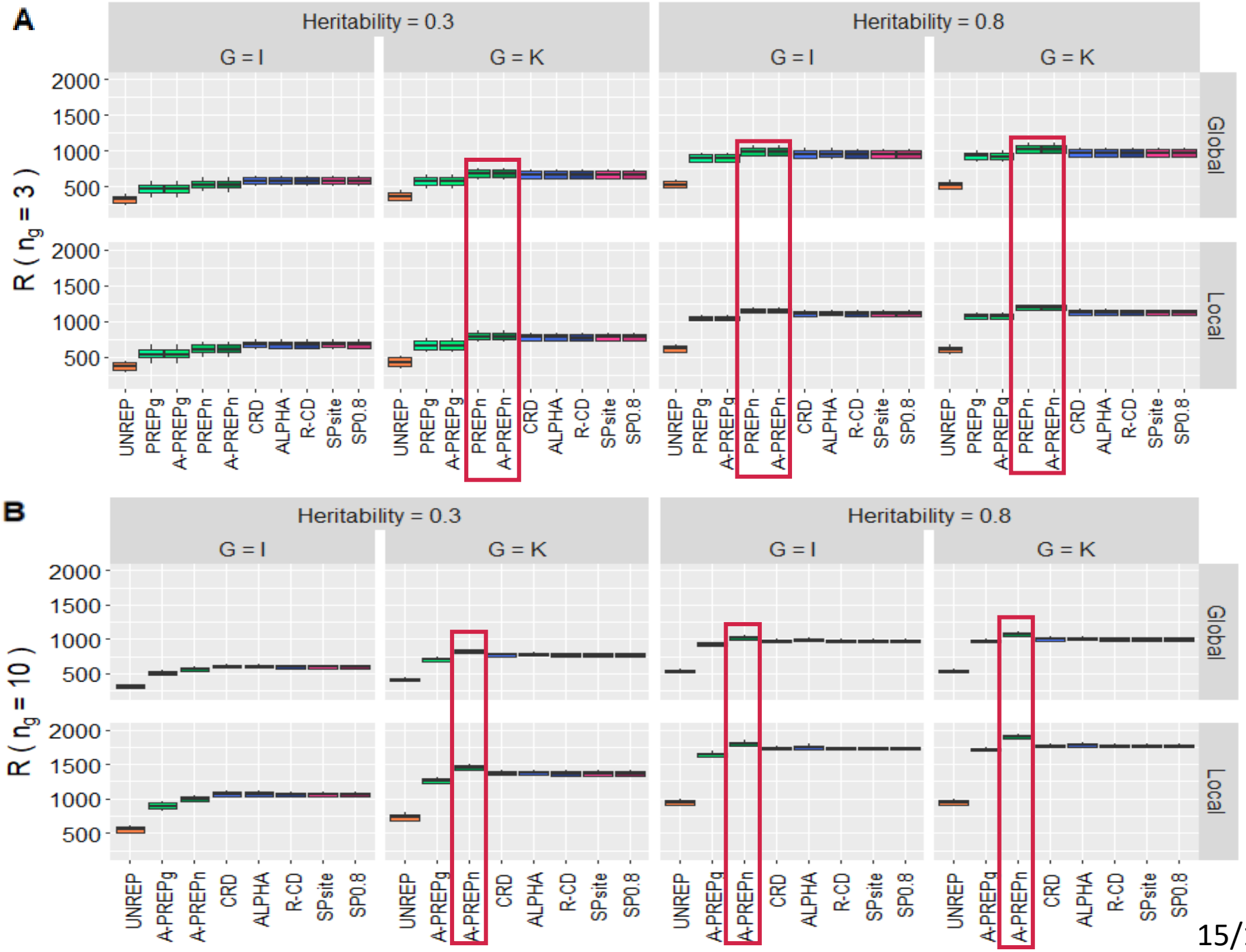

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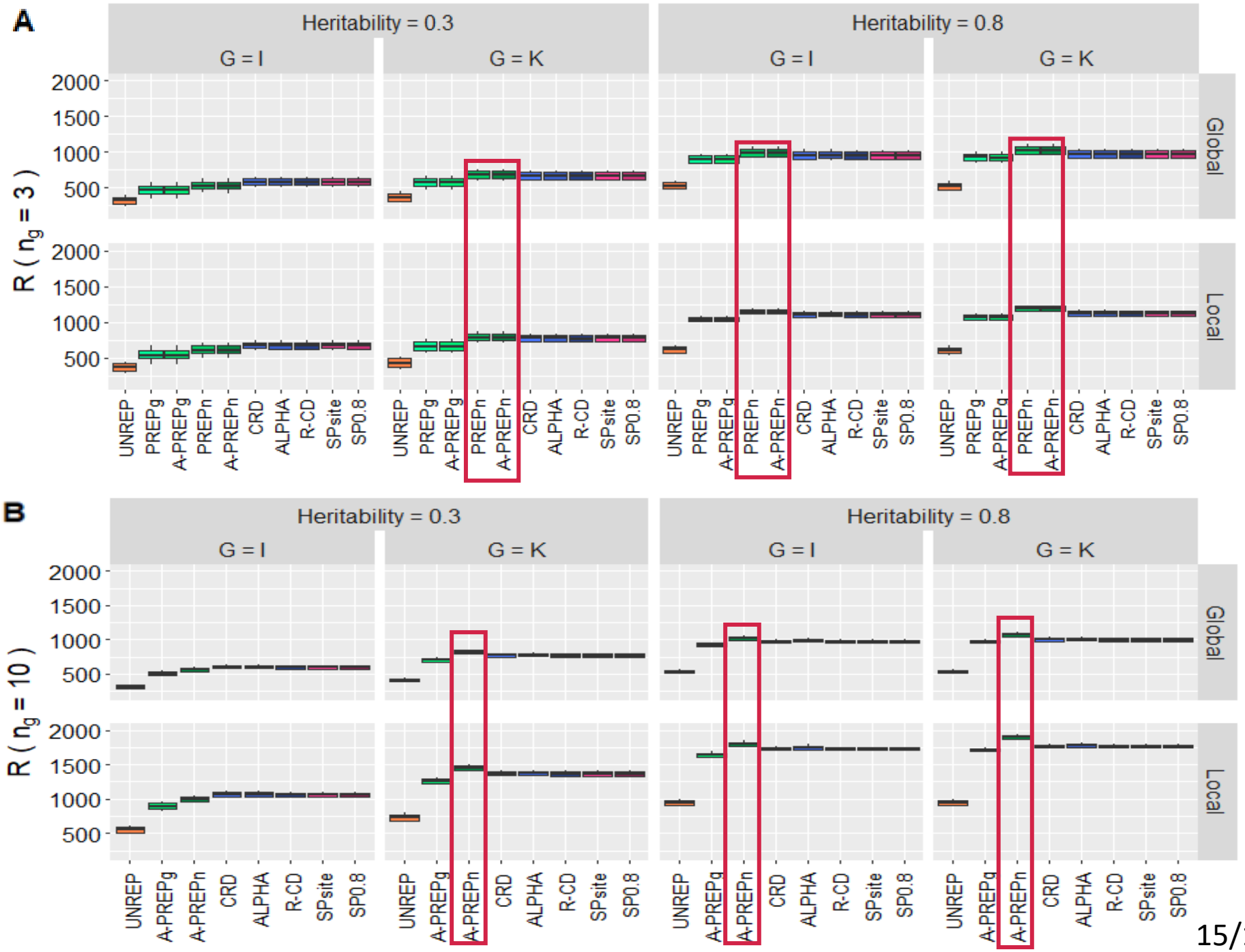
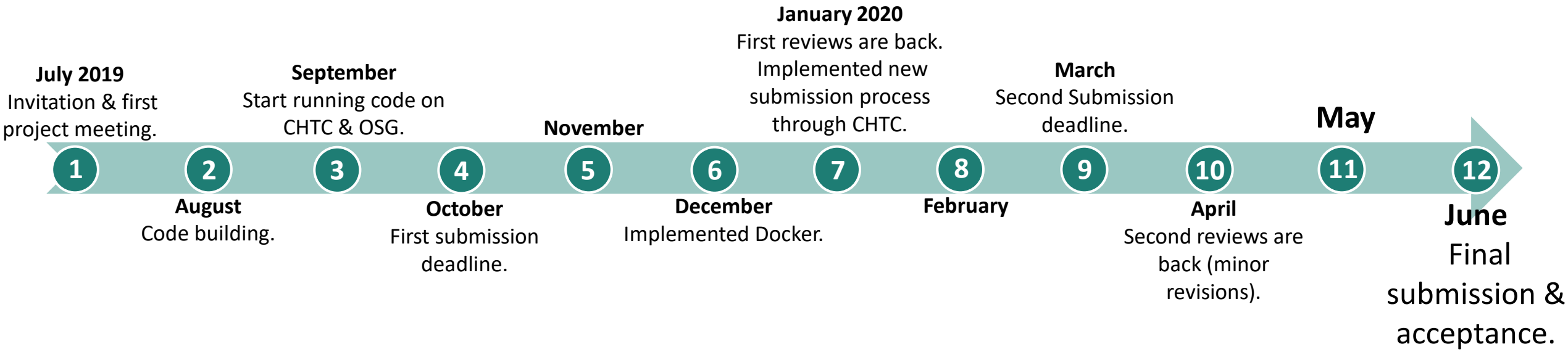
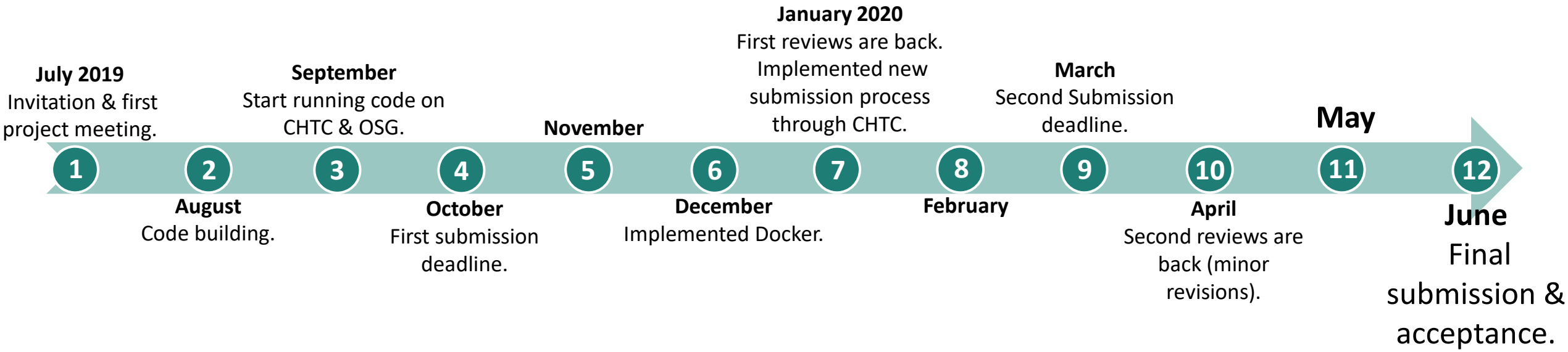
~130 K hours





- Final reflections



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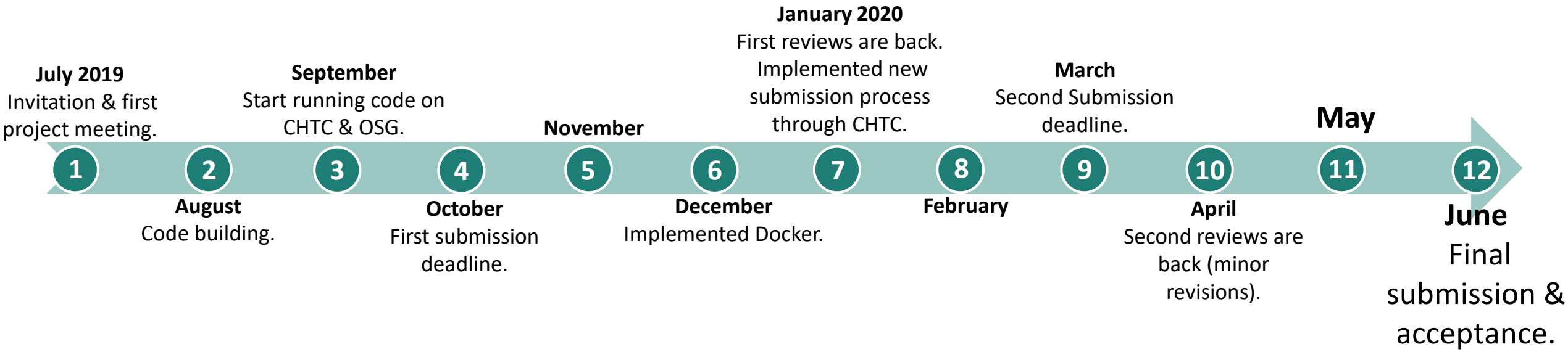
  - Huge undertaking.



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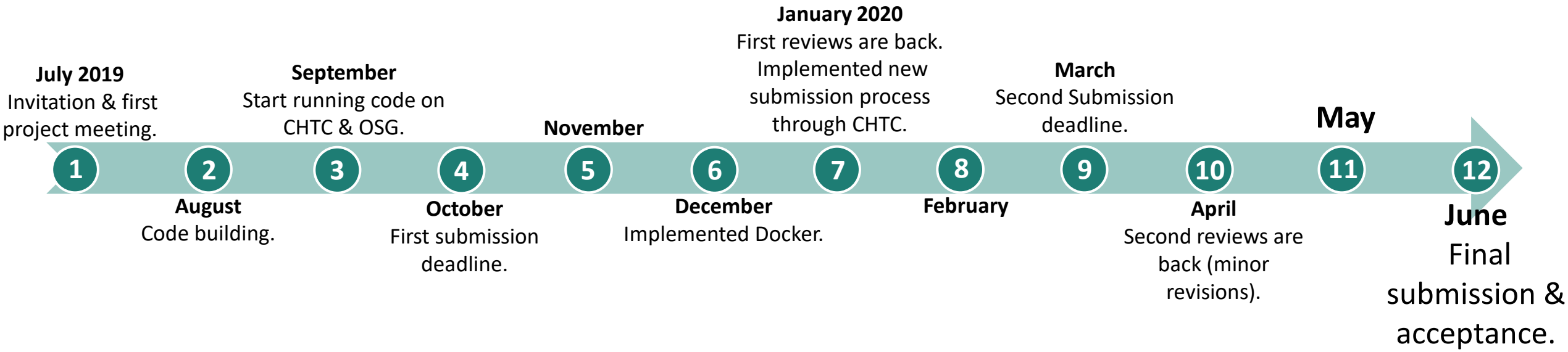
  - Deadlines were our largest battle.



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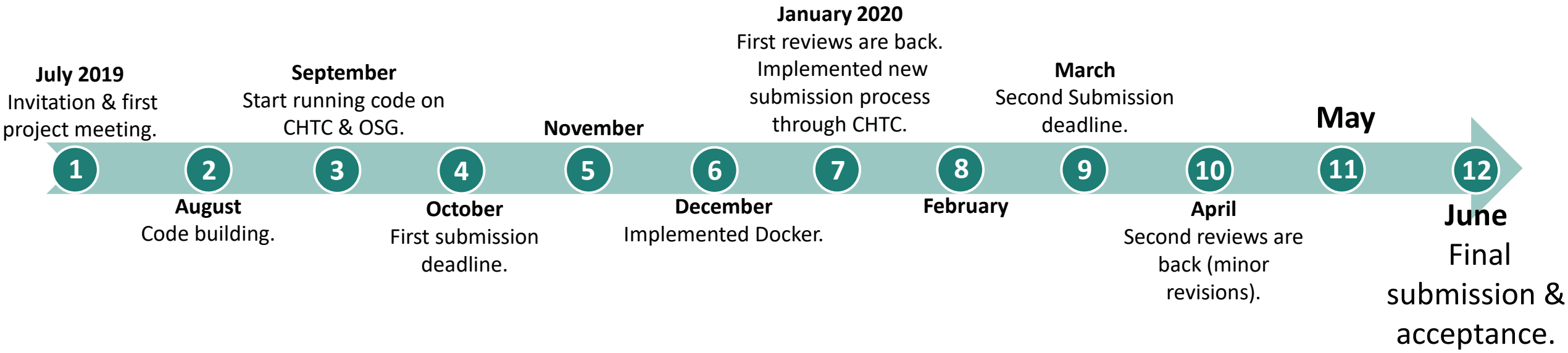

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  - Interactive help sessions were very useful.
    - OSG User School
    - Office hours

Supplementary materials for this article are available at https://doi.org/10.1007/s13253-020-00406-2.

Do Spatial Designs Outperform Classic Experimental Designs?

Raegan HOEFLER, Pablo GONZÁLEZ- BARRIOS, Madhav BHATTA, Jose A. R. NUNES, Ines BERRO, Rafael S. NALIN, Alejandra BORGES, Eduardo COVARRUBIAS, Luis DIAZ- GARCIA, Martin QUINCKE, and Lucia GUTIERREZ

Controlling spatial variation in agricultural field trials is the most important step to compare treatments efficiently and accurately. Spatial variability can be controlled at the experimental design level with the assignment of treatments to experimental units and at the modeling level with the use of spatial corrections and other modeling strategies. The goal of this study was to compare the efficiency of methods used to control spatial variation in a wide range of scenarios using a simulation approach based on real wheat data. Specifically, classic and spatial experimental designs with and without a two-dimensional autoregressive spatial correction were evaluated in scenarios that include differing experimental unit sizes, experiment sizes, relationships among genotypes, genotype by environment interaction levels, and trait heritabilities. Fully replicated designs outperformed partially and unreplicated designs in terms of accuracy; the alpha-lattice incomplete block design was best in all scenarios of the medium-sized experiments. However, in terms of response to selection, partially replicated experiments that evaluate large population sizes were superior in most scenarios. The AR1 × AR1 spatial correction had little benefit in most scenarios except for the medium-sized experiments with the largest experimental unit size and low GE. Overall, the results from this study provide a guide to researchers designing and analyzing large field experiments.
Supplementary materials accompanying this paper appear online.

Key Words: Experimental design; Autoregressive process; Prediction accuracy; Response to selection; Spatial correction; Randomization-based experimental designs.

DOI: 10.1007/s13253-020-00406-2

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Acknowledgements

Authors

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Eduardo Covarrubias
Luis Diaz-Garza
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Lucia Gutierrez

Gutierrez Lab

CHTC and OSG Team

Lauren Michael
Christina Koch
Jess Vera

OSG CONNECT

CENTER FOR HIGH THROUGHPUT COMPUTING

WISCONSIN
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