GPU-parallel Gibbs sampling of a hierarchical model of hybrid vigor in RNA-seq experiments

Will Landau

Iowa State University

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Biological background
- DNA and RNA
- Central dogma
- Examples of gene regulation
- RNA-seq
- Hybrid vigor

The model

The Gibbs sampler
- Gibbs steps
- Estimated heterosis probabilities
- GPU parallelism

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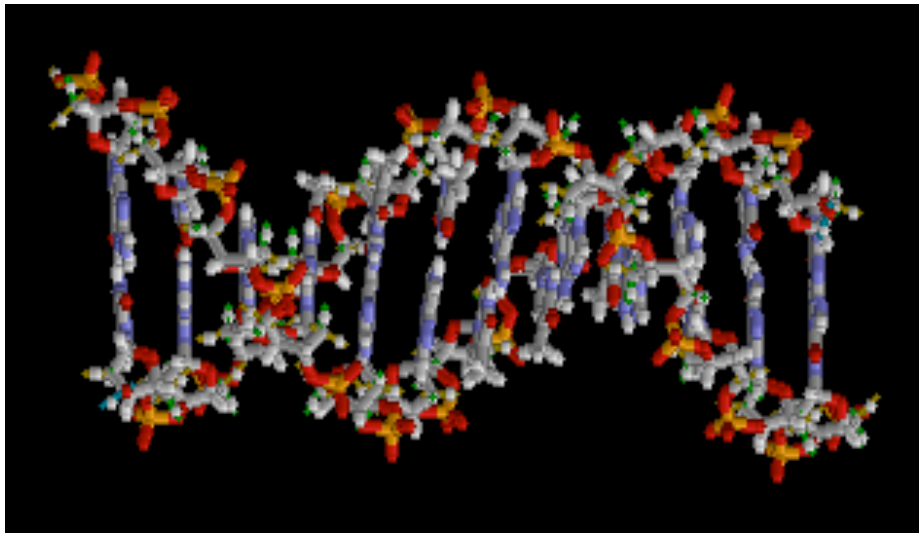
DNA



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... GTGCATCTGACTCCTGAGGAGAAG ...
... CACGTAGACTGAGGACTCCTCTTC ...
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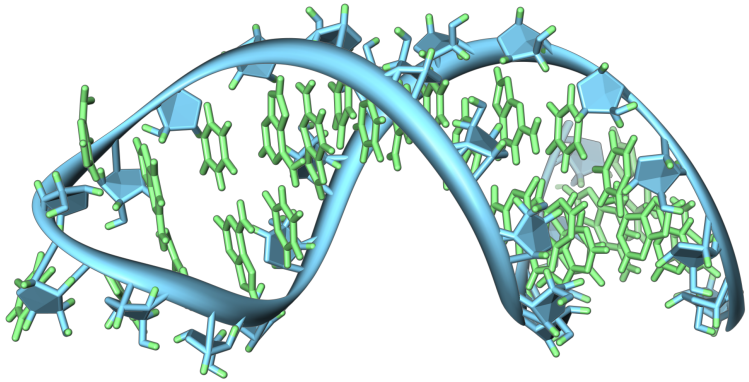
RNA



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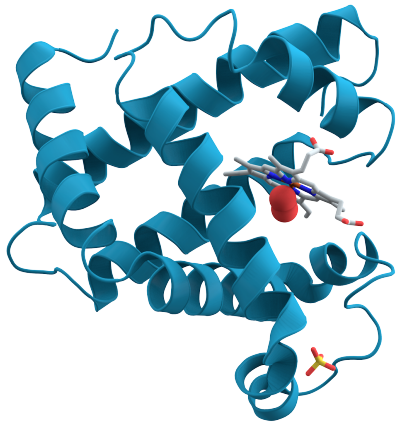
Proteins



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Central dogma: how organisms make proteins

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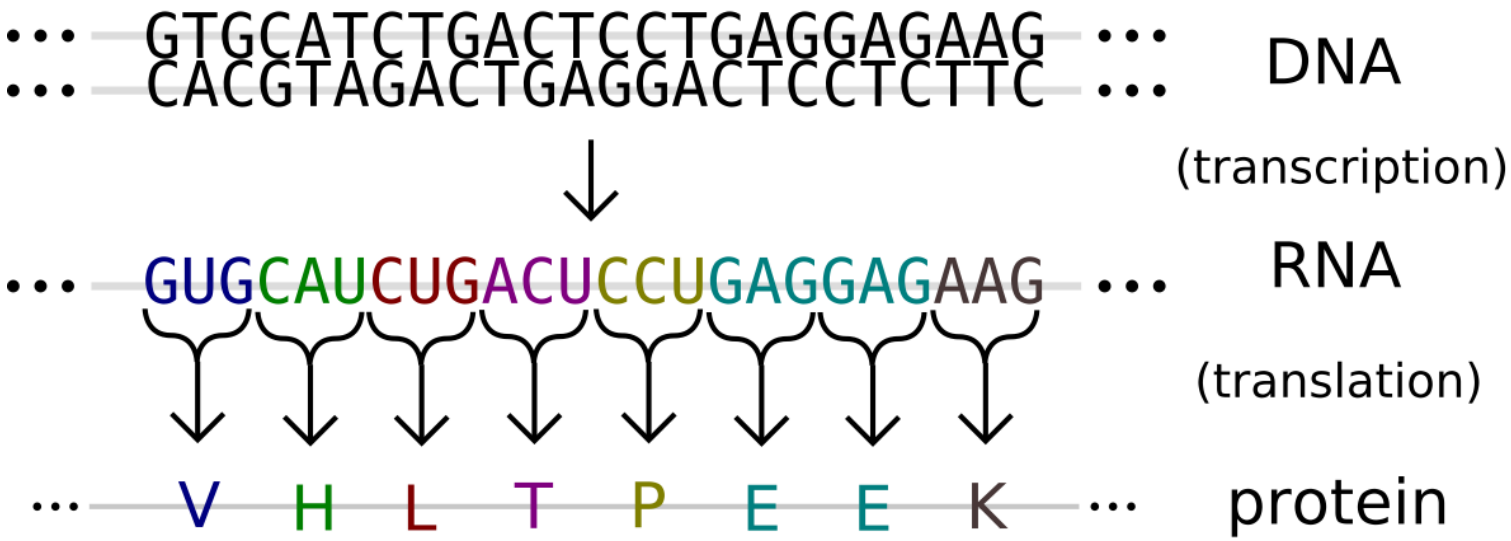
Central dogma of genetics



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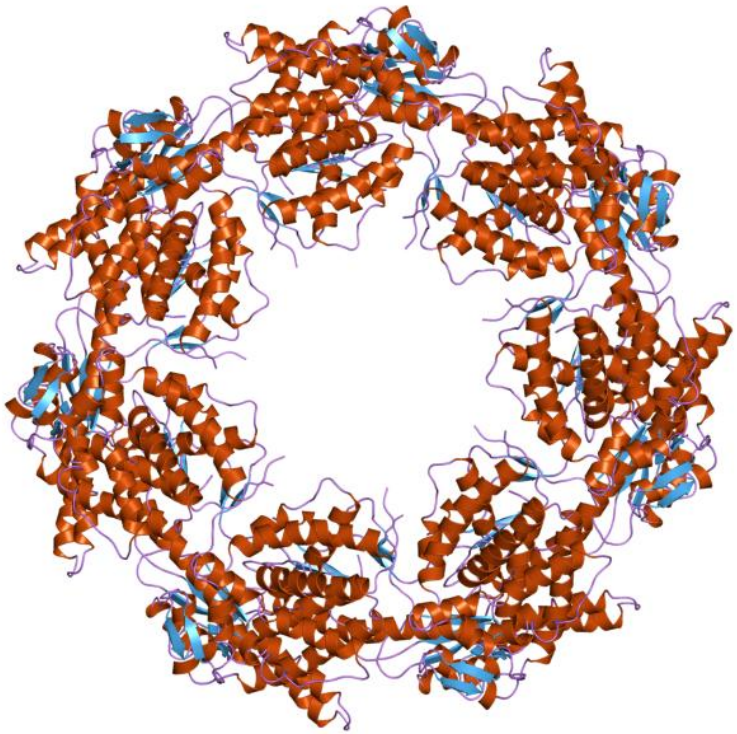
HSP60

- HSP = heat shock protein.
- Prevent heat damage to other proteins.



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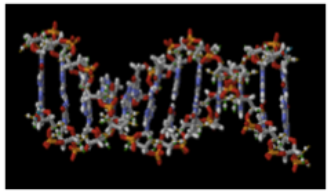
Temperature spike triggers HSP60 production.

HSP60 Gene



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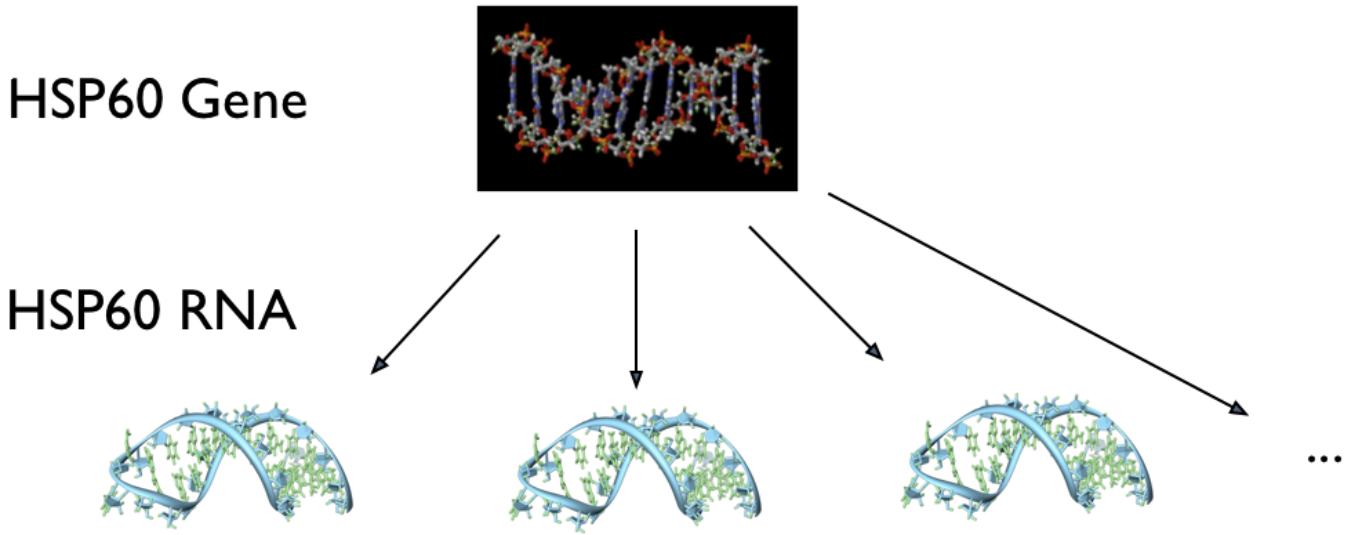
Temperature spike causes HSP60 expression.



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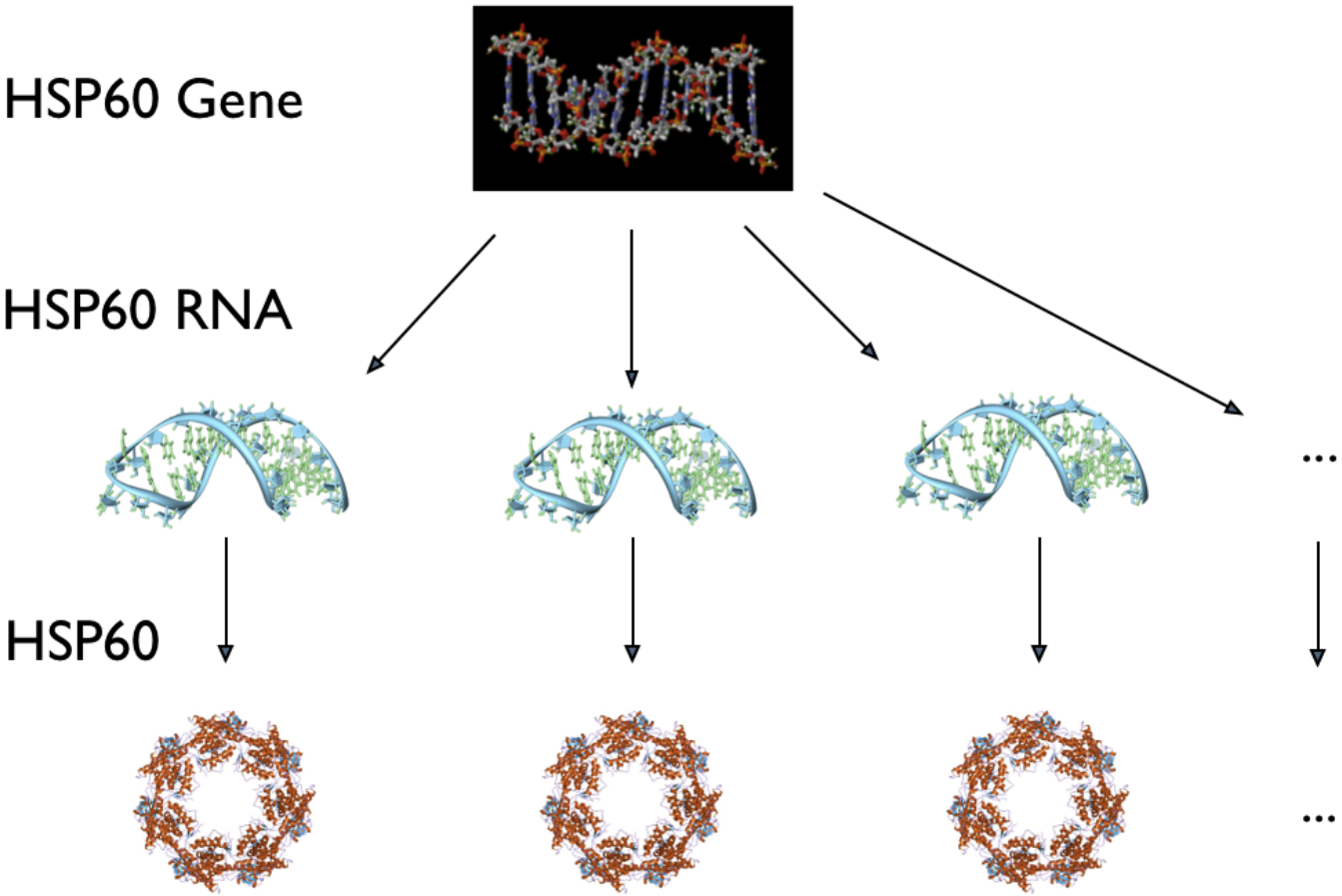

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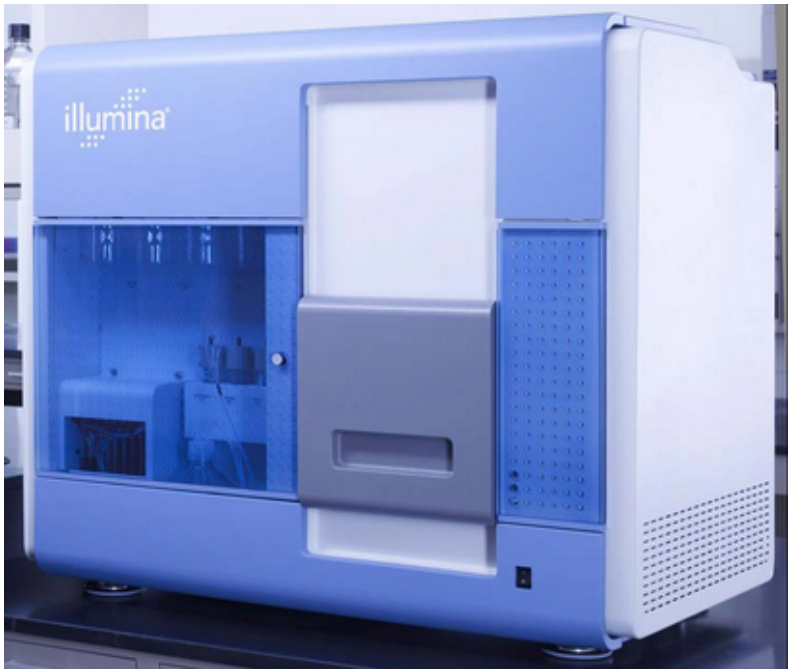
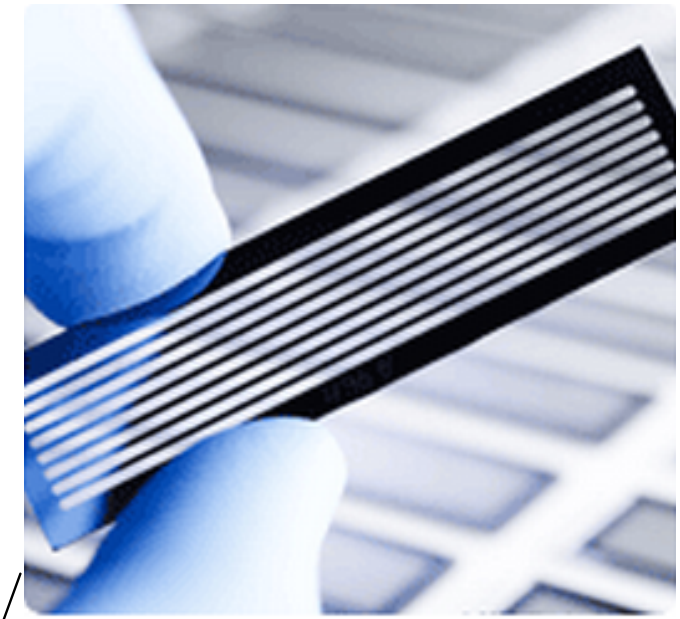
RNA-seq

- RNA sequencing: measure gene expression using relative abundance of RNA.
- Illumina Genome Analyzer:





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RNA-seq data: counts of amplified RNA fragments

	Treatment 1			Treatment 2		Treatment 3	
Gene 1	100	225	0	70	279	300	106
Gene 2	0	1	1	50	501	2	7
Gene 3	3	4	2	700	900	0	0
Gene 4	893	400	760	5	5	1000	513
...	...	...	...	...	...	...	...
Gene 34897	10	13	6	819	761	902	912

- Goal: use RNA-seq to study hybrid vigor (heterosis).

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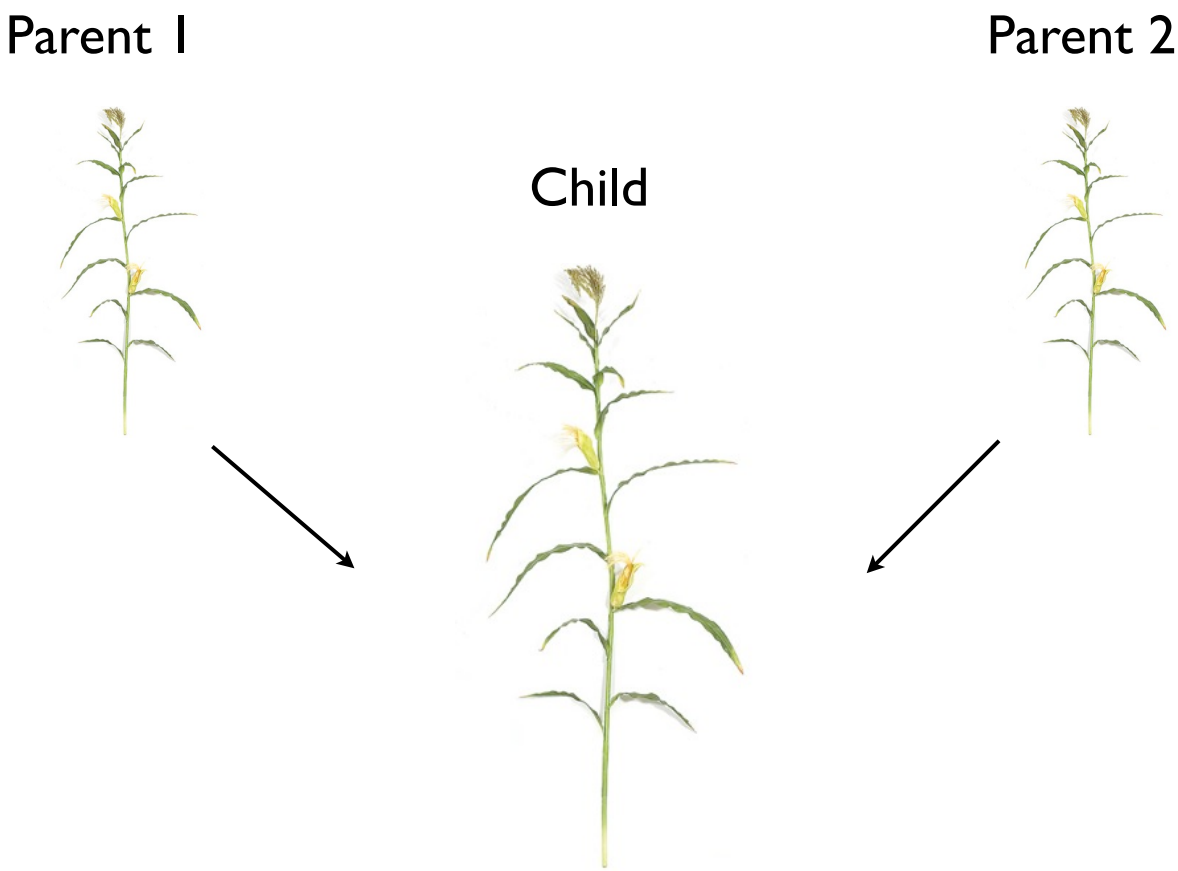
High-parent heterosis: child's trait surpasses both parents



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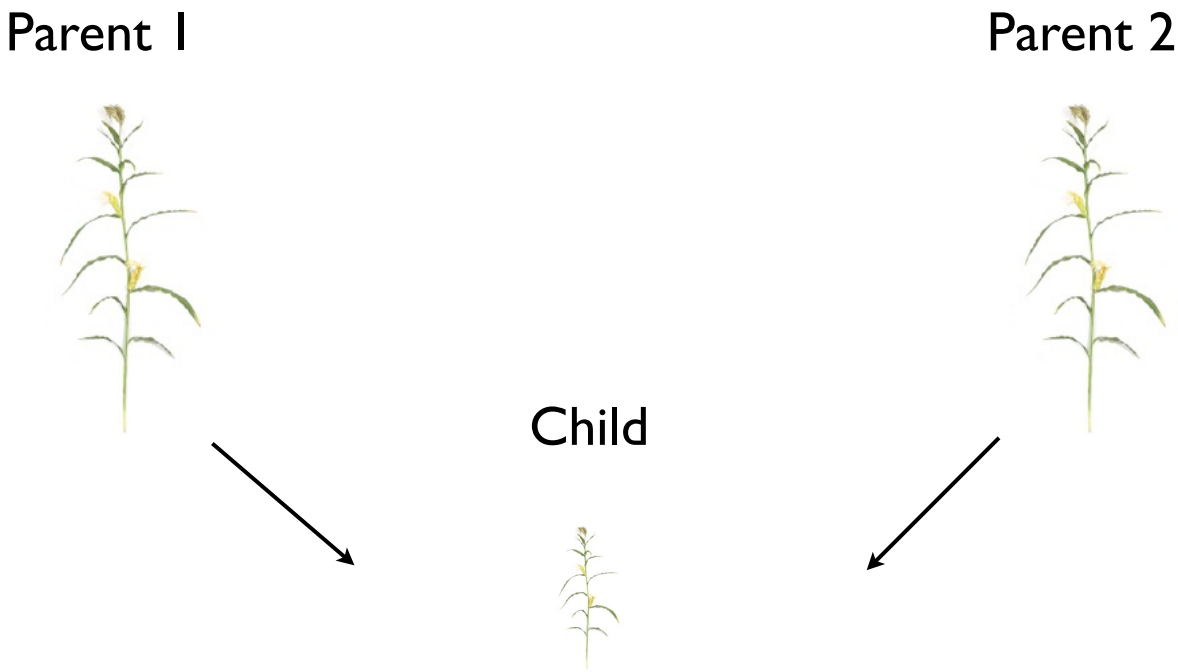
Low-parent heterosis: child's trait is weaker than in each parent



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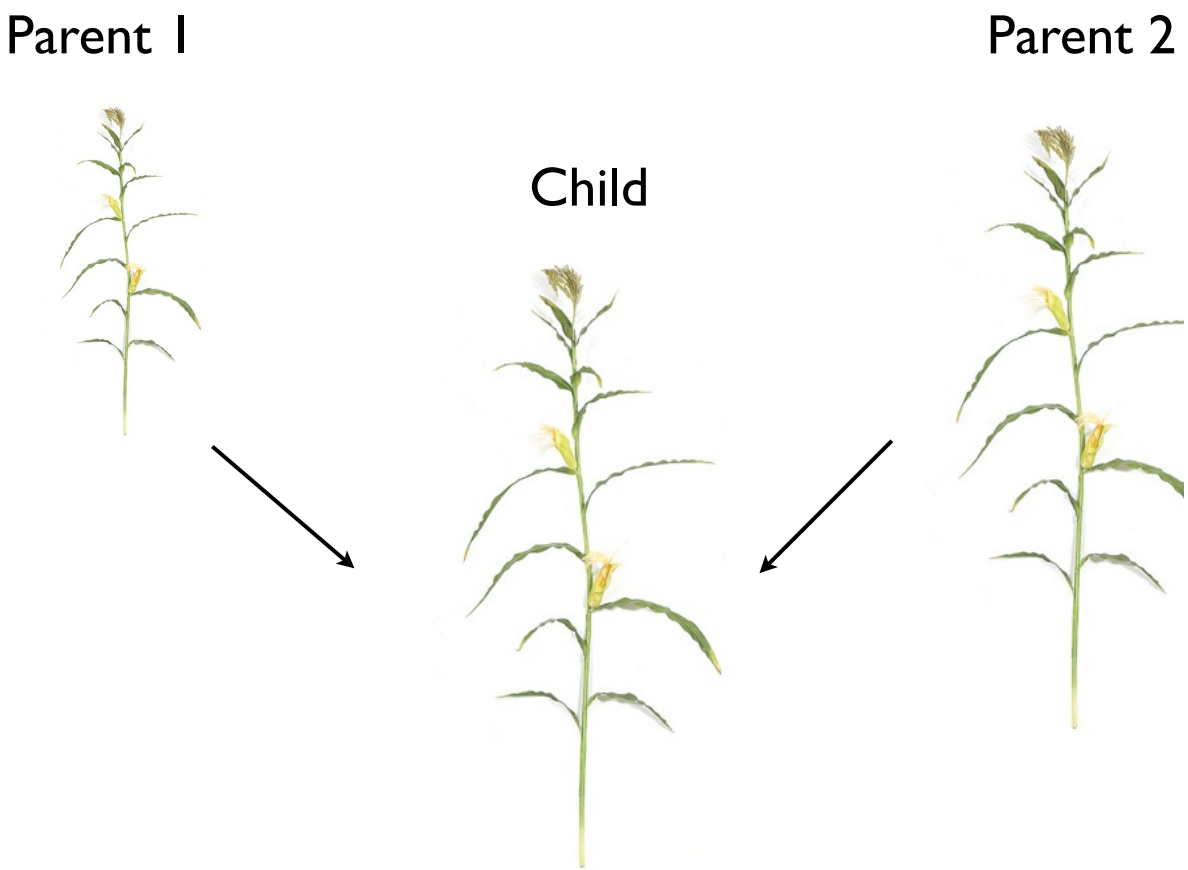
Mid-parent heterosis: child's trait is different than average of parents



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High-parent heterosis in gene expression

	Parent 1			Child		Parent 2	
Gene 1	100	225	0	70	279	300	106
Gene 2	0	1	1	50	501	2	7
Gene 3	3	4	2	700	900	0	0
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$$\mu(n, \phi_g, \alpha_g, \delta_g) = \begin{cases} \phi_g - \alpha_g & \text{sample } n \text{ from parent 1} \\ \phi_g + \delta_g & \text{sample } n \text{ from child} \\ \phi_g + \alpha_g & \text{sample } n \text{ from parent 2} \end{cases}$$

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

$$c_n \overset{\text{ind}}{\sim} \text{N}(0, \sigma_c^2)$$

$$\sigma_c \sim \text{U}(0, \sigma_{c0})$$

$$\varepsilon_{g,n} \overset{\text{ind}}{\sim} \text{N}(0, \eta_g^2)$$

$$\eta_g^2 \overset{\text{ind}}{\sim} \text{Inv-Gamma}\left(\text{shape} = \frac{d}{2}, \text{ rate} = \frac{d\tau^2}{2}\right)$$

$$d \sim \text{U}(0, d_0)$$

$$\tau^2 \sim \text{Gamma}(\text{shape} = a_\tau, \text{rate} = b_\tau)$$

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$$\phi_g \overset{\text{ind}}{\sim} \text{N}(\theta_\phi, \sigma_\phi^2)$$

$$\theta_\phi \sim \text{N}(0, \gamma_\phi^2)$$

$$\sigma_\phi \sim \text{U}(0, \sigma_{\phi 0})$$

$$\alpha_g \overset{\text{ind}}{\sim} \pi_\alpha^{1-I(\alpha_g)}[(1-\pi_\alpha)\text{N}(\theta_\alpha, \sigma_\alpha^2)]^{I(\alpha_g)}$$

$$\theta_\alpha \sim \text{N}(0, \gamma_\alpha^2)$$

$$\sigma_\alpha \sim \text{U}(0, \sigma_{\alpha 0})$$

$$\pi_\alpha \sim \text{Beta}(a_\alpha, b_\alpha)$$

$$\delta_g \overset{\text{ind}}{\sim} \pi_\delta^{1-I(\delta_g)}[(1-\pi_\delta)\text{N}(\theta_\delta, \sigma_\delta^2)]^{I(\delta_g)}$$

$$\theta_\delta \sim \text{N}(0, \gamma_\delta^2)$$

$$\sigma_\delta \sim \text{U}(0, \sigma_{\delta 0})$$

$$\pi_\delta \sim \text{Beta}(a_\delta, b_\delta)$$

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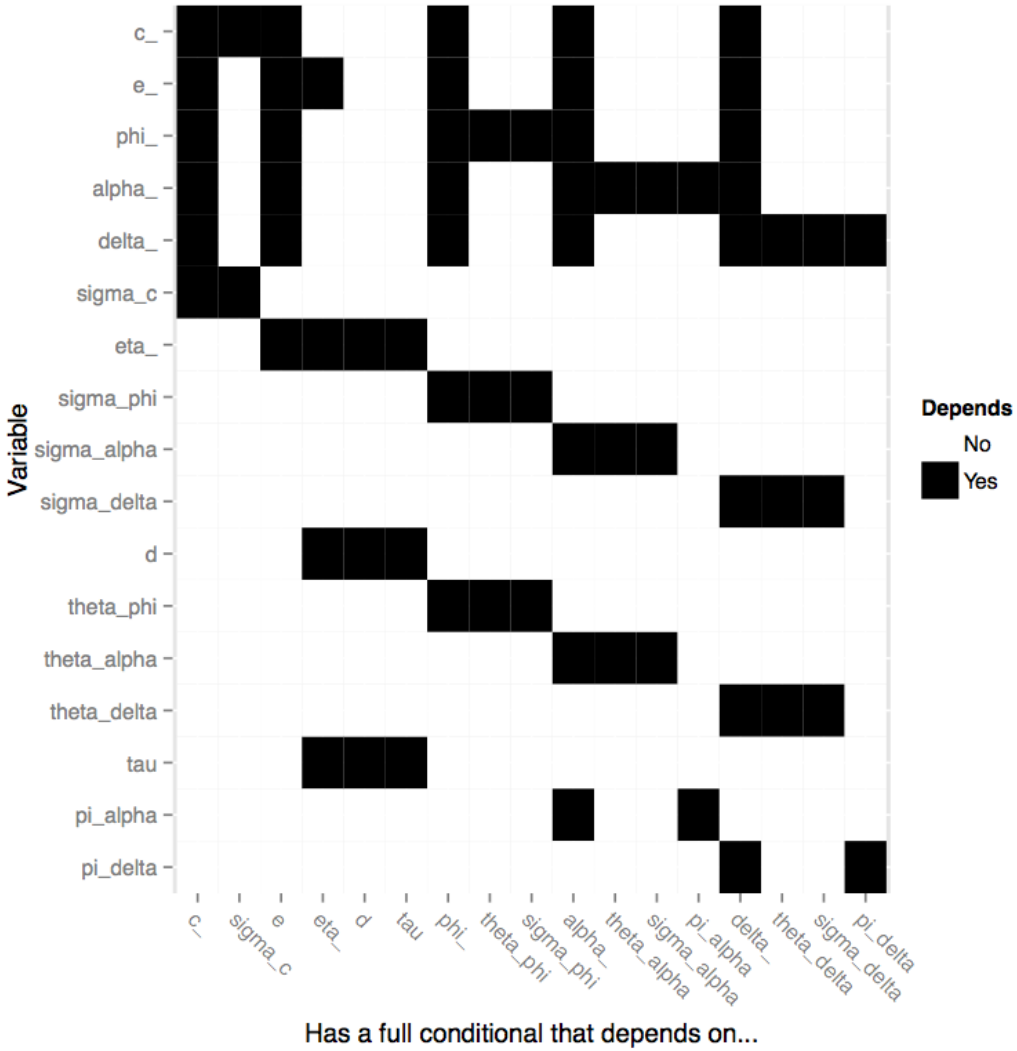
Partition parameters by conditional independence.



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Use these partitions as Gibbs steps.

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

- From the appropriate full conditional distributions, sample the following:

1. $c_1, \ldots, c_N$
2. $\tau, \pi_\alpha, \pi_\delta$
3. $d, \theta_\phi, \theta_\alpha, \theta_\delta$
4. $\sigma_c, \sigma_\phi, \sigma_\alpha, \sigma_\delta, \eta_1^2, \ldots, \eta_G^2$
5. $\varepsilon_{1,1}, \varepsilon_{1,2}, \ldots, \varepsilon_{1,N}, \varepsilon_{2,N}, \ldots, \varepsilon_{G,N}$
6. $\phi_1, \ldots, \phi_G$
7. $\alpha_1, \ldots, \alpha_G$
8. $\delta_1, \ldots, \delta_G$

- and then repeat.

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$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

Consider one chain with M iterations.

$$P(\text{high-parent heterosis in gene } g) \approx \frac{1}{M} \sum_{i=1}^{M} I(\delta_g^{(i)} > |\alpha_g^{(i)}|)$$

$$P(\text{low-parent heterosis in gene } g\ ) \approx \frac{1}{M} \sum_{i=1}^{M} I(\delta_g^{(i)} < -|\alpha_g^{(i)}|)$$

$$P(\text{mid-parent heterosis in gene } g\ ) \approx \frac{1}{M} \sum_{i=1}^{M} I(|\delta_g^{(i)}| < |\alpha_g^{(i)}|)$$

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Tons of opportunity for GPU parallelism across genes!

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

- Sample in parallel:
  - ϕ_g's
  - α_g's
  - δ_g's
  - $\varepsilon_{g,n}$'s
  - η_g's

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Example: ϕ_g's

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

$$\phi_g \overset{\text{ind}}{\sim} \text{N}(\theta_\phi, \sigma_\phi^2)$$

$$\theta_\phi \sim \text{N}(0, \gamma_\phi^2)$$

$$\sigma_\phi \sim \text{U}(0, \sigma_{\phi 0})$$

- Using parallel random walk Metropolis steps, sample the ϕ_g's from their full conditional distributions,

$$p(\phi_g \mid \cdots) \propto \exp\left(\sum_{n=1}^{N} [y_{g,n} \cdot \mu(n, \phi_g, \alpha_g, \delta_g) - \exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g))] - \frac{(\phi_g - \theta_\phi)^2}{2\sigma_\phi^2}\right)$$

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$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

- Use **parallel reductions** to calculate sufficient statistics for:
  - c_n's
  - τ, d
  - θ_ϕ, θ_α, θ_δ
  - σ_ϕ, σ_α, σ_δ, σ_c
  - π_α, π_δ

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Pairwise summation: an example reduction

- Let's take the pairwise sum of the vector,

$$(5, 2, -3, 1, 1, 8, 2, 6)$$

using 1 block of 4 threads.

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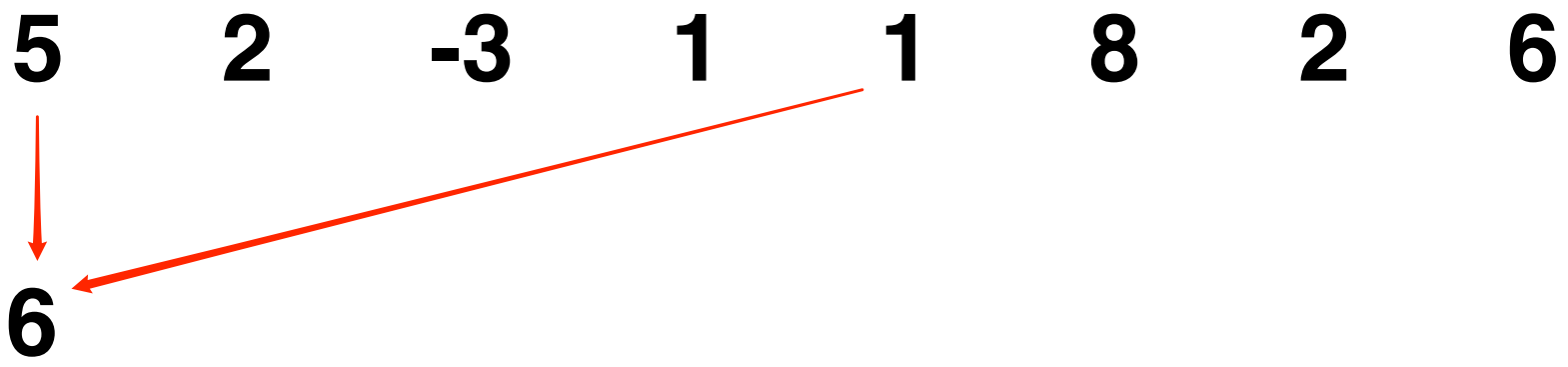

Thread 0

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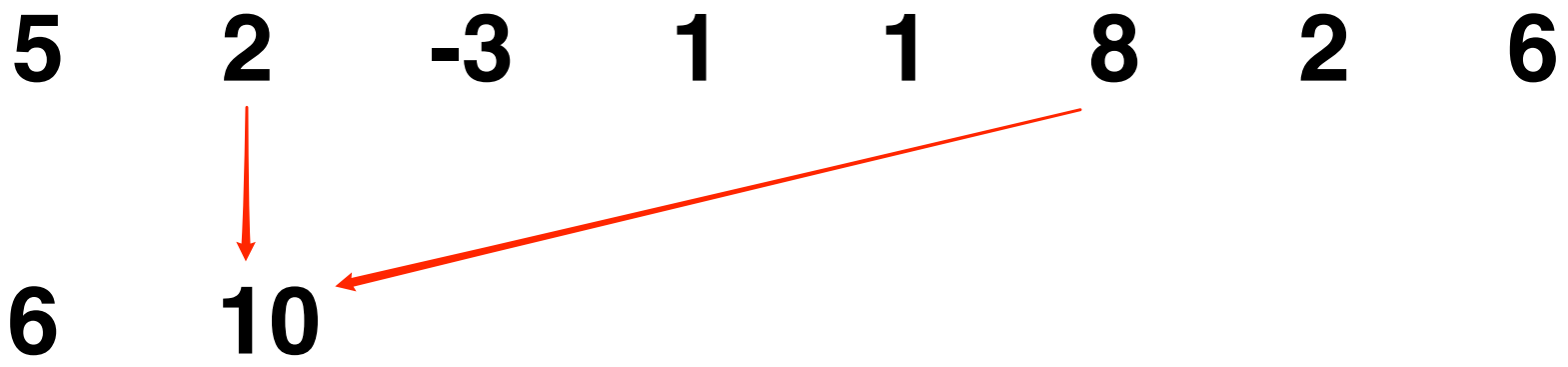

Thread 1

GPU-parallel Gibbs sampling of a hierarchical model of hybrid vigor in RNA-seq experiments

Will Landau

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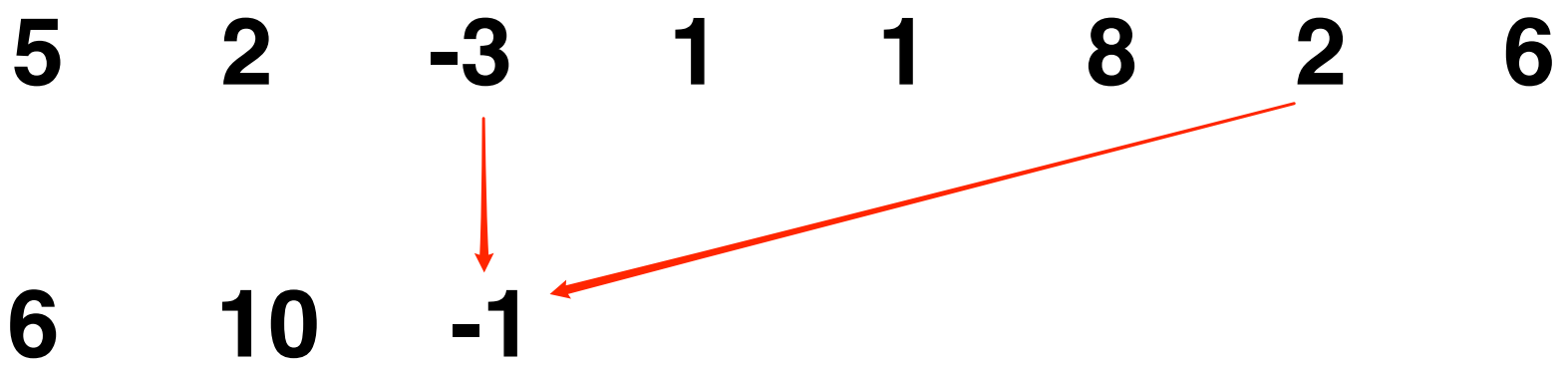

Thread 2

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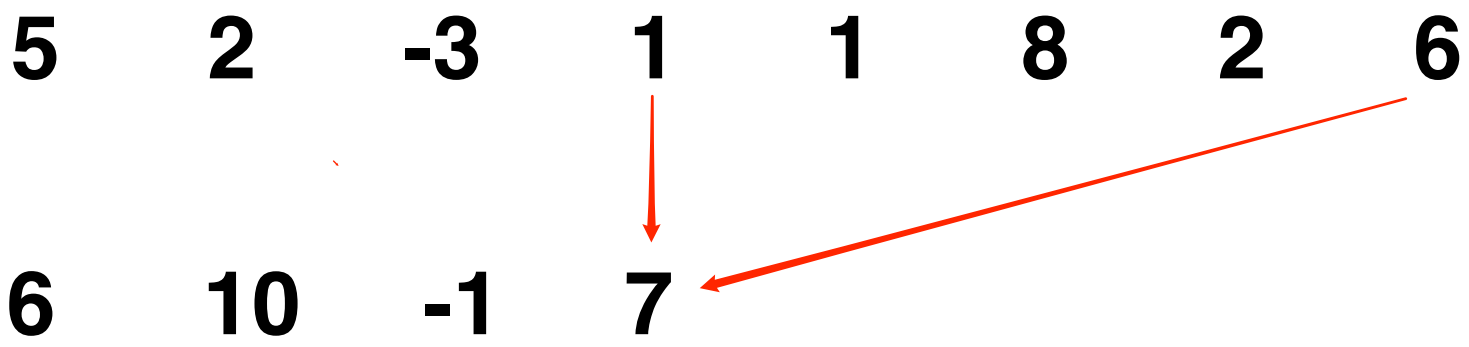

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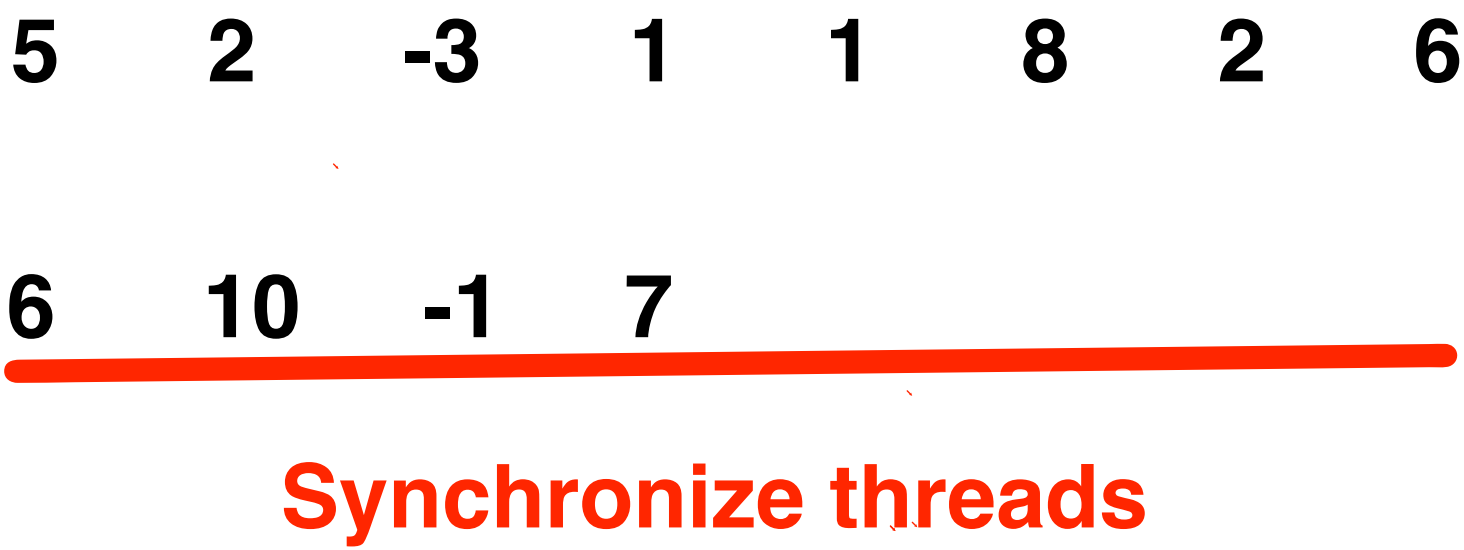

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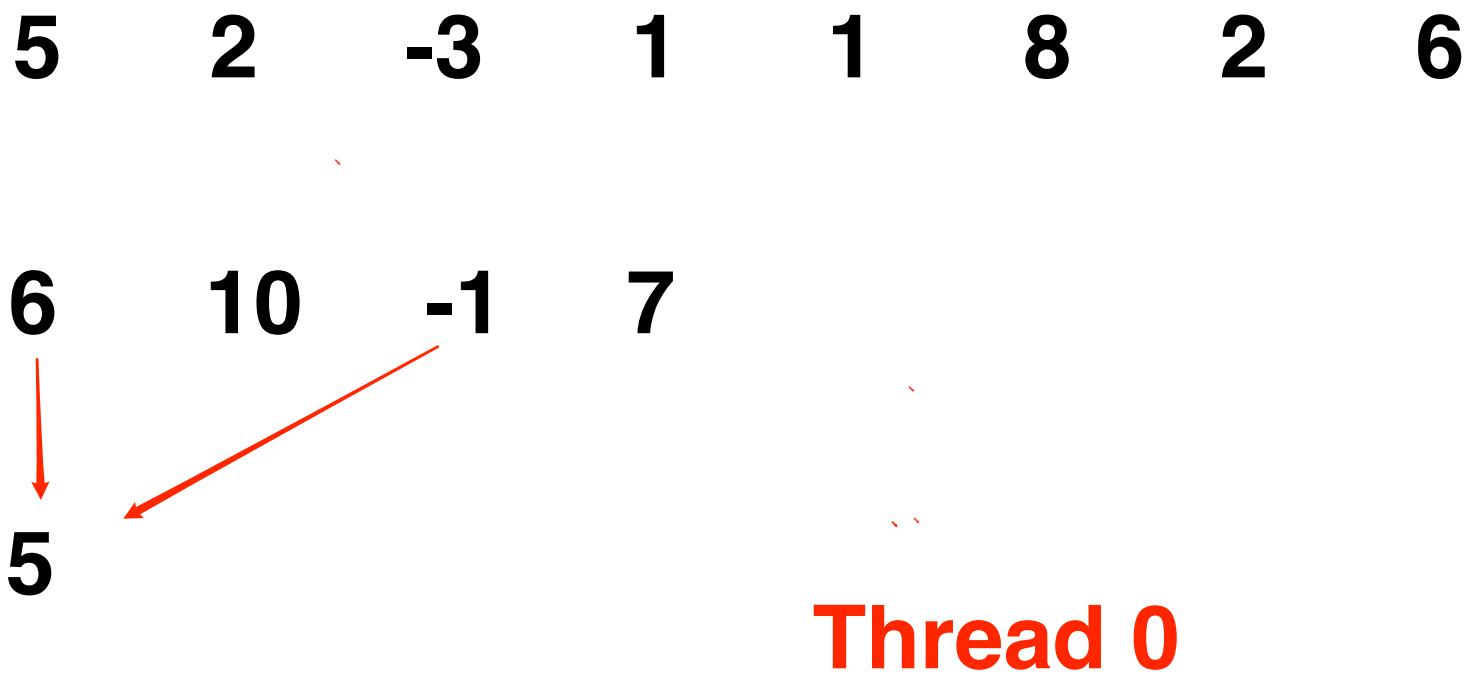

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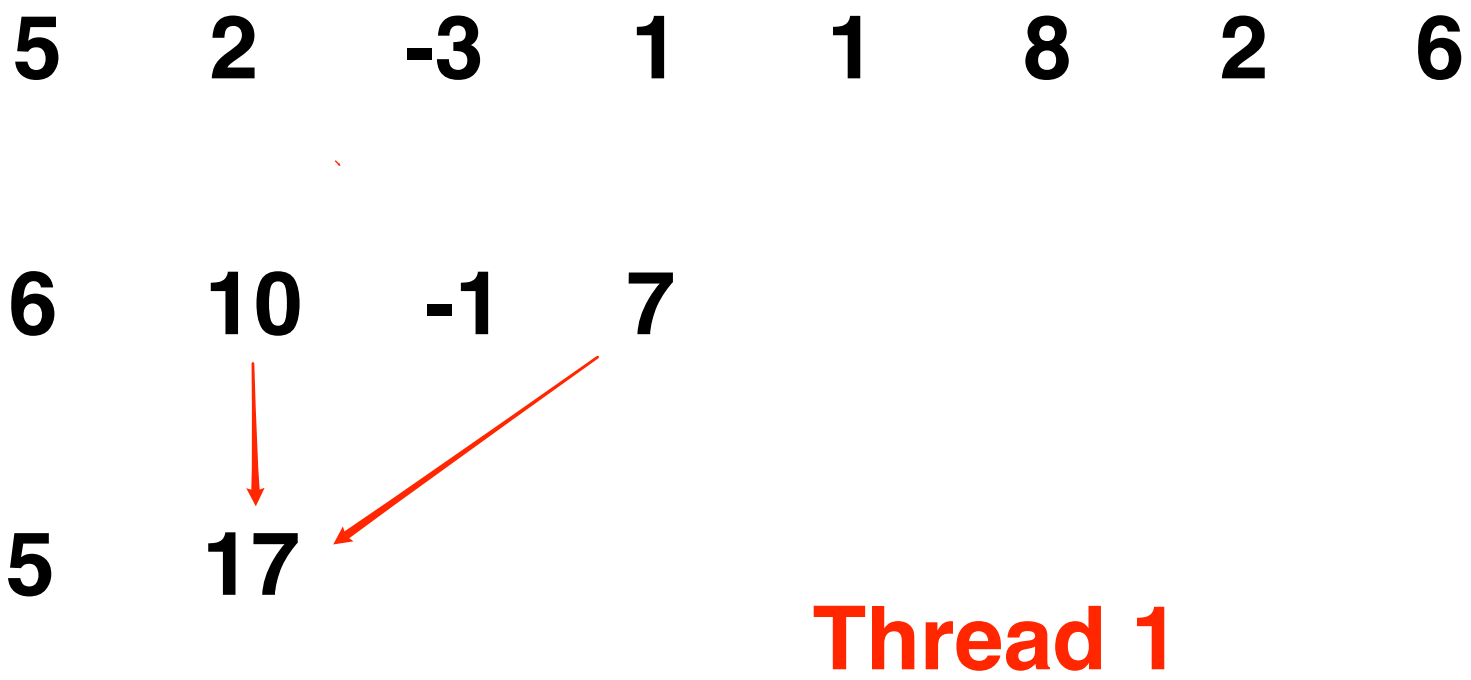

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5 2 -3 1 1 8 2 6

6 10 -1 7

5 17

Synchronize Threads

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Example: τ^2

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

$$\varepsilon_{g,n} \overset{\text{ind}}{\sim} \text{N}(0, \eta_g^2)$$

$$\eta_g^2 \overset{\text{ind}}{\sim} \text{Inv-Gamma}\left(\text{shape} = \frac{d}{2}\ ,\ \text{rate} = \frac{d \cdot \tau^2}{2}\right)$$

$$d \sim \text{U}(0, d_0)$$

$$\tau^2 \sim \text{Gamma}(\text{shape} = a_\tau, \text{rate} = b_\tau)$$

$$p(\tau^2 \mid \cdots)$$

$$= \text{Gamma}\left(\text{shape} = a_\tau + \frac{Gd}{2}\ ,\ \text{rate} = b_\tau + \frac{d}{2}\sum_{g=1}^{G}\frac{1}{\eta_g^2}\right)$$

- Using a parallel reduction (NVIDIA's CUDA C/C++ `Thrust` library), calculate the sufficient statistic:

$$\sum_{g=1}^{G}\frac{1}{\eta_g^2}$$

- Use an efficient rejection sampler to sample τ^2.

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Example: d

$$y_{g,n} \overset{\text{ind}}{\sim} \text{Poisson}(\exp(c_n + \varepsilon_{g,n} + \mu(n, \phi_g, \alpha_g, \delta_g)))$$

$$\varepsilon_{g,n} \overset{\text{ind}}{\sim} \text{N}(0, \eta_g^2)$$

$$\eta_g^2 \overset{\text{ind}}{\sim} \text{Inv-Gamma}\left(\text{shape} = \frac{d}{2}\ ,\ \text{rate} = \frac{d \cdot \tau^2}{2}\right)$$

$$d \sim \text{U}(0, d_0)$$

$$\tau^2 \sim \text{Gamma}(\text{shape} = a_\tau, \text{rate} = b_\tau)$$

$$p(d \mid \cdots) \propto \Gamma(d/2)^{-G} \left(\frac{d \cdot \tau^2}{2}\right)^{Gd/2} \left(\prod_{g=1}^{G} \eta_g^2\right)^{-(d/2+1)} \exp\left(-\frac{d \cdot \tau^2}{2} \sum_{g=1}^{G} \frac{1}{\eta_g^2}\right) I(0 < d < d_0)$$

- Using parallel reductions (NVIDIA's CUDA C/C++ `Thrust` library), calculate the sufficient statistics:

$$\prod_{g=1}^{G} \eta_g^2 \qquad \sum_{g=1}^{G} \frac{1}{\eta_g^2}$$

- Use a random-walk metropolis step to sample d.

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- Ordinary C and GPU-accelerated versions, along with an R package wrapper, are available for download at https://github.com/wlandau/heterosis.
- Time for a demo...

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Thanks for coming.

- Slides and video will be available at http://will-landau.com/research.html.

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Sources

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