More Data + Heterogeneous Compute = Fractured Workflows: Why mathematical and computational structure matter more than ever

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- **Global : ZB/year (EB/day scale)**

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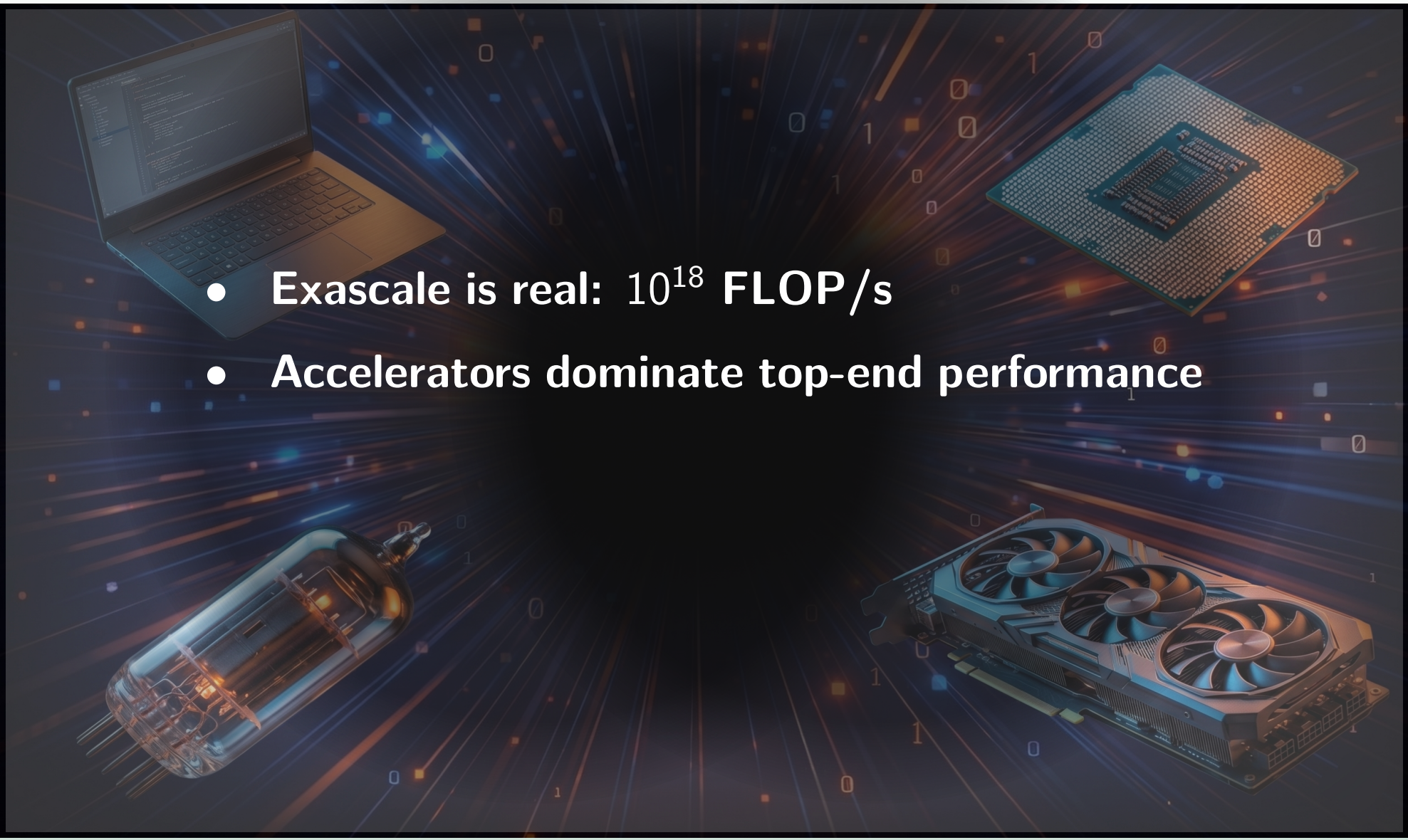
Compute explosion



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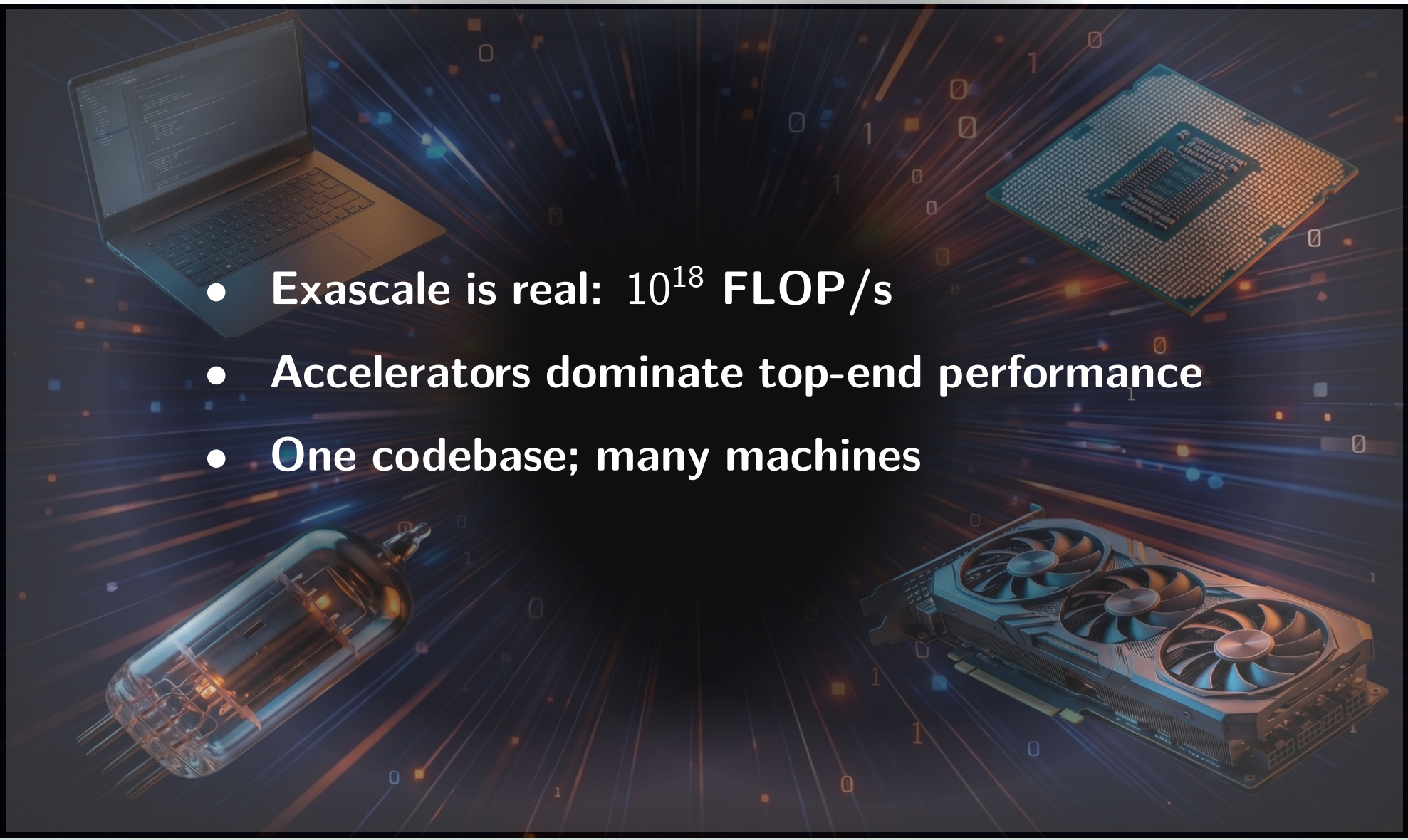

- **Exascale is real: 10^{18} FLOP/s**
- **Accelerators dominate top-end performance**
- **One codebase; many machines**

A maxim

As machines become more powerful, the efficiency of algorithms grows more important, not less.

— Maxim 9, Trefethen, Maxims about numerical mathematics, science, computers, and life on earth

Another maxim

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our expectations for speed, fidelity, and reliability.

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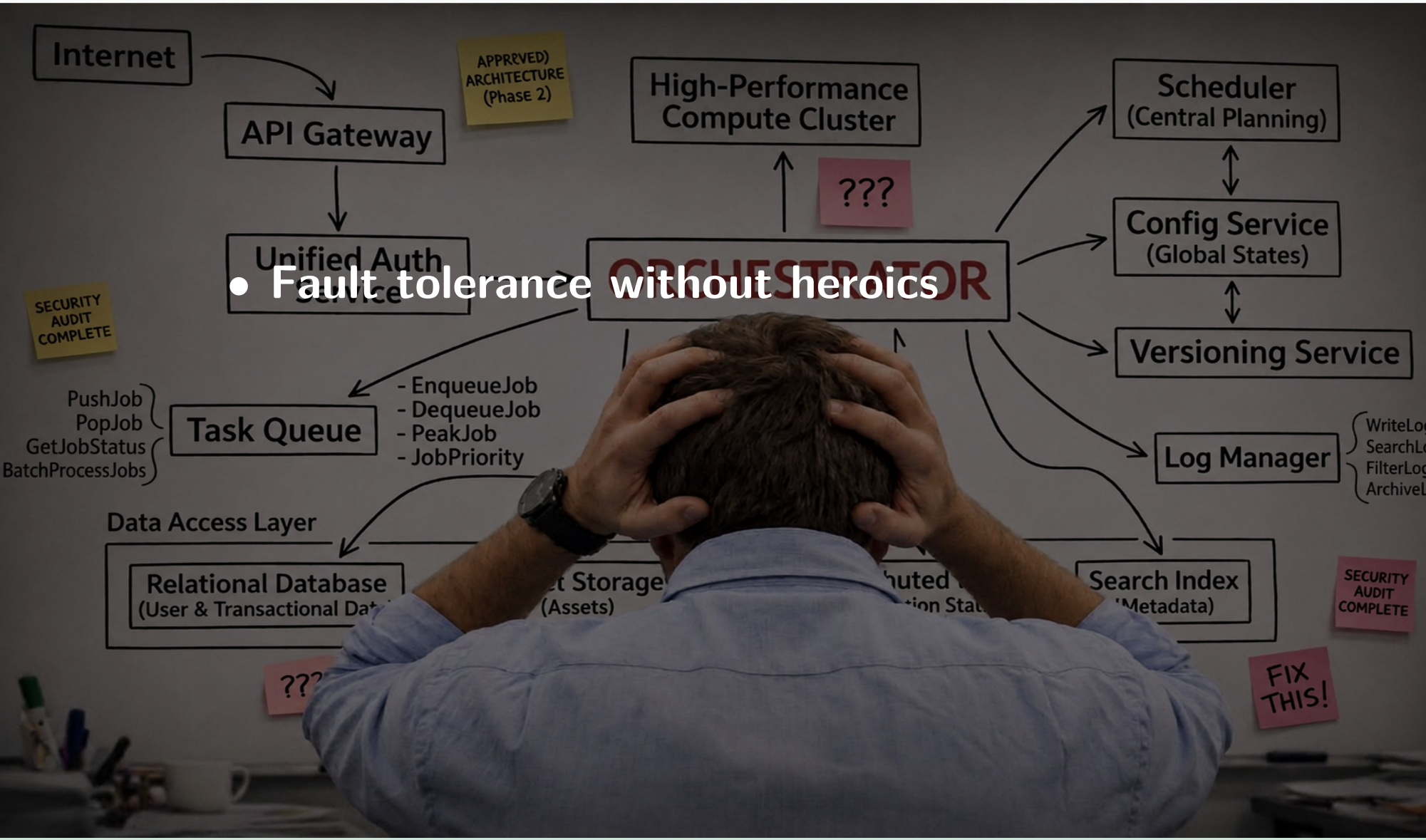

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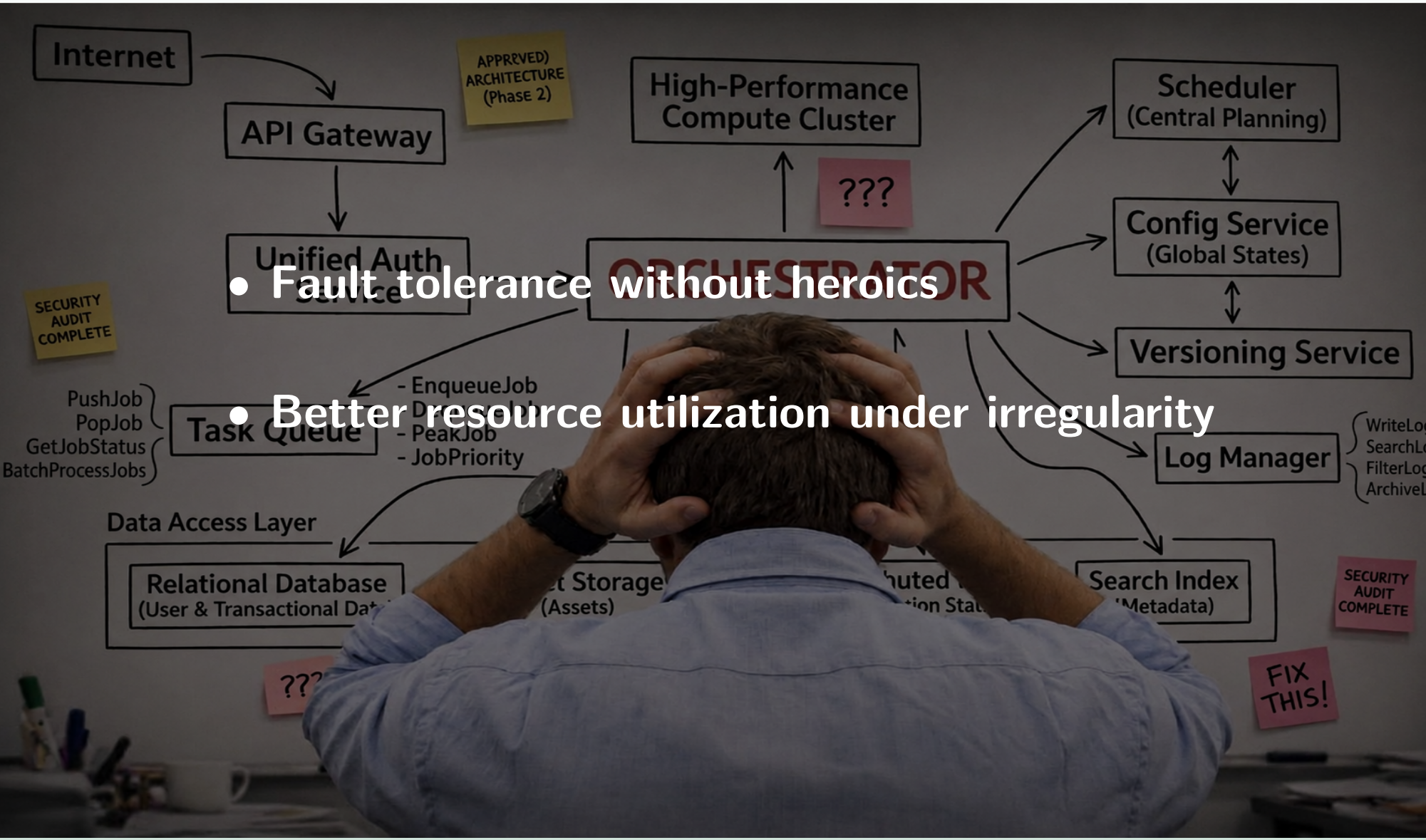

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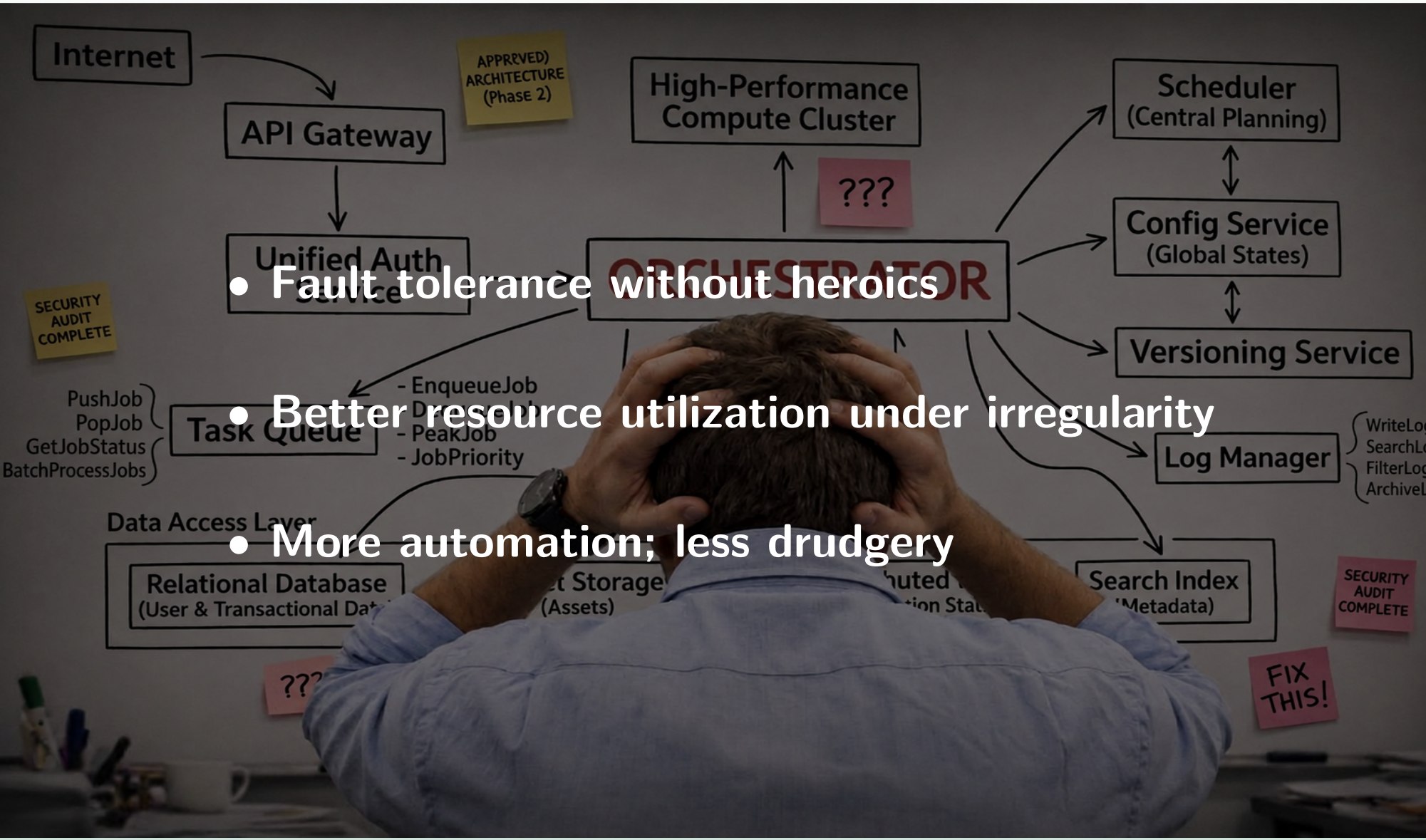

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- **Better resource utilization under irregularity**
- **More automation; less drudgery**

When things get messy

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- split computationally

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Useful instincts. Dangerous habits.

What splitting can break mathematically

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Fractional-step methods for differential equations

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Fractional-step methods for differential equations

- split processes
- advance them independently
- hope the important interactions survive

What are we really signing up for?

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- split the work
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Structure should holistically drive the method.

Example: Niederer benchmark

Monodomain model of cardiac electrophysiology

PDE:

$$\chi C_m \frac{\partial v}{\partial t} = \nabla \cdot \left(\frac{\lambda}{1+\lambda} \sigma_i \nabla v \right) - \chi \Big(I_{\text{ion}}(\mathbf{s}, v) + I_{\text{stim}}(t, \mathbf{x}) \Big)$$

$$\frac{\partial \mathbf{s}}{\partial t} = \mathbf{g}(\mathbf{s}, v)$$

Discretized and split:

$$\begin{bmatrix} \dot{\mathbf{V}} \\ \dot{\mathbf{S}} \end{bmatrix} = \begin{bmatrix} \frac{1}{C_m \chi} \sigma^{-1} \mathbf{D} \mathbf{V} \\ 0 \end{bmatrix} + \begin{bmatrix} -\frac{1}{C_m} (I_{\text{ion}}(\mathbf{S}, \mathbf{V}) + I_{\text{stim}}(t)) \\ \mathbf{G}(\mathbf{S}, \mathbf{V}) \end{bmatrix}$$

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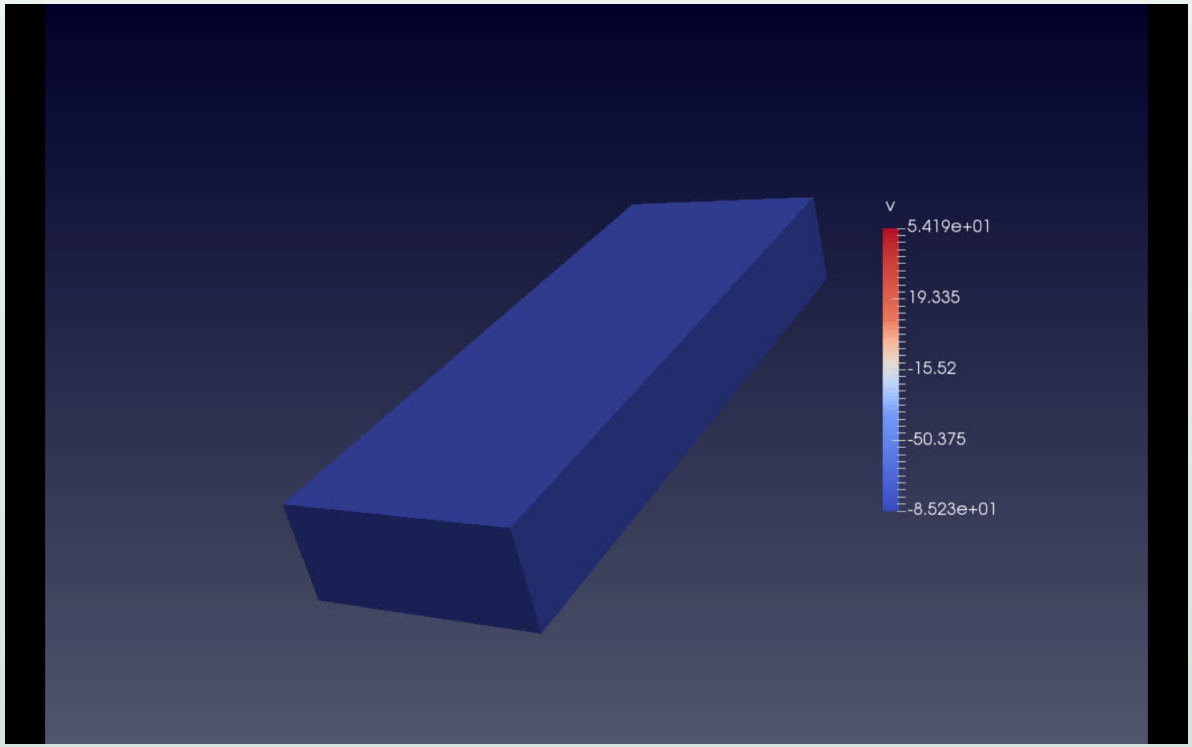
Example: Niederer benchmark details

Domain: $\mathbf{x} \in 0.3 \text{ cm} \times 0.7 \text{ cm} \times 2 \text{ cm}$; $t \in [0, 40]$ ms

Spatial discretization: central FD, $\Delta x = \Delta y = \Delta z = 0.05$ cm

Cell model: Ten Tusscher–Panfilov (19 ODEs; stiff)

Target $< 5\%$ $[\text{MRMS}]_v$ error



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Splitting is (by far) not the end of method design.

A framework for splitting method design

Theorem

An N-split FSRK method has an extended Butcher tableau

$$\begin{array}{c|c:c:c:c|c:c:c:c} \mathbf{c}^{[1]} & \mathbf{c}^{[2]} & \dots & \mathbf{c}^{[N]} & \mathbf{A}^{[1]} & \mathbf{A}^{[2]} & \dots & \mathbf{A}^{[N]} \\ \hline & & & & \mathbf{b}^{[1]} & \mathbf{b}^{[2]} & \dots & \mathbf{b}^{[N]} \end{array}$$

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The test equation $\frac{\mathrm{d}y}{\mathrm{d}t} = \sum_{\ell=1}^{N} \lambda^{[\ell]} y$ *leads to the stability function*

$$R(z^{[1]}, z^{[2]}, \dots, z^{[N]}) = \prod_{k=1}^{s} \prod_{\ell=1}^{N} R_k^{[\ell]}(\alpha_k^{[\ell]} z^{[\ell]}),$$

where $z^{[\ell]} = \Delta t \lambda^{[\ell]}$ *and* $R_k^{[\ell]}(z^{[\ell]})$ *is the stability function of the Runge–Kutta method at stage* k *applied to operator* ℓ.

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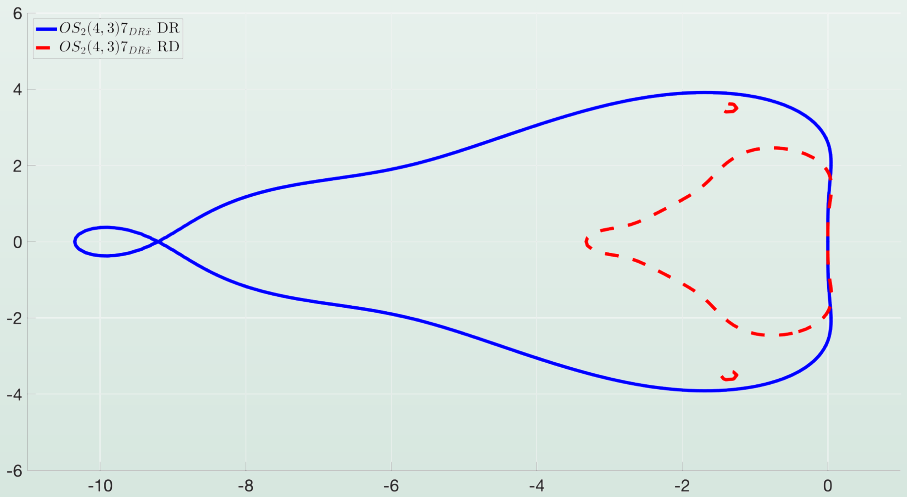
- sub-integrator choice matters
- operator ordering matters
- stability design enables larger stable steps

A framework for splitting method design

For the Niederer benchmark,

$$\lambda^{[D]} \approx -1.92,\ \lambda^{[R]} \approx -1260 \quad \Longrightarrow \quad |\lambda^{[D]}| \approx 0.001\,|\lambda^{[R]}|$$



Niederer benchmark: performance

Same split. Different design. Different outcome.

method	DR ordering			RD ordering		
	Δt	CPU (s)	$[\text{MRMS}]_v$	Δt	CPU (s)	$[\text{MRMS}]_v$
Ruth	2.8×10^{-3}	8831	6.7×10^{-4}	6.2×10^{-3}	3962	3.9×10^{-4}
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Theory-guided design turns into speed.

Example 2: Strength-Interval Curves

- measures recovery of tissue excitability
- useful for studying vulnerability to re-entry
- can be measured using S1–S2 protocol
- plot stimulus threshold for second wave vs. S2 interval
- one SI curve = many threshold solves

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The workflow is the bottleneck.

What is an SI curve, really?

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One SI curve is a family of related event-location problems.

- find minimum S1 to establish initial wave
- for each interval, find minimum S2 that re-triggers wave
- each threshold found by bisection

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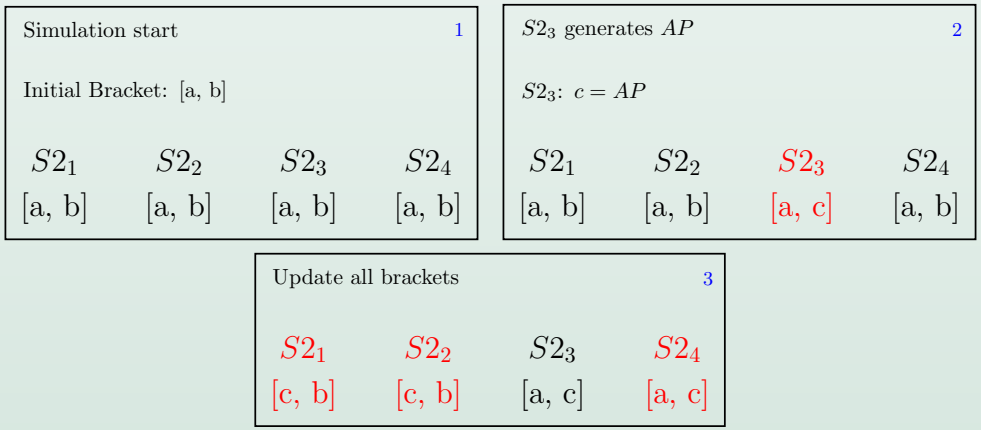

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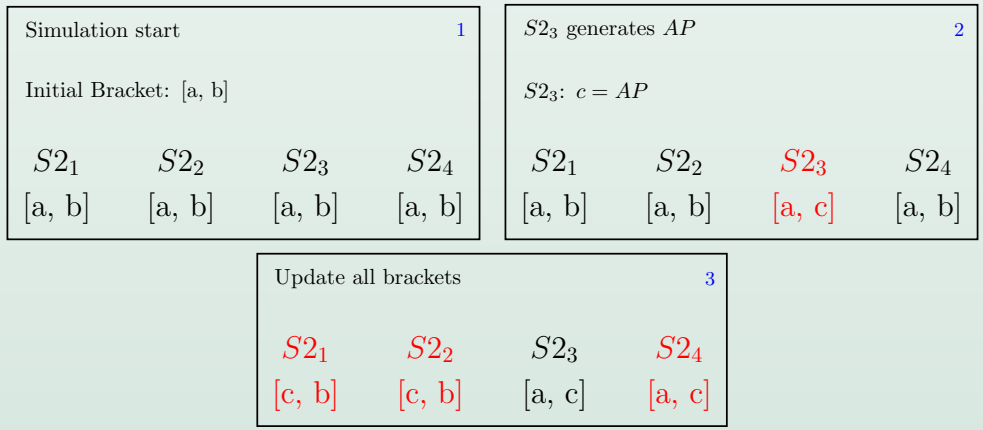

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A painful fit for traditional computing.

Actors: a different orchestration model

The actor model of concurrent computation.

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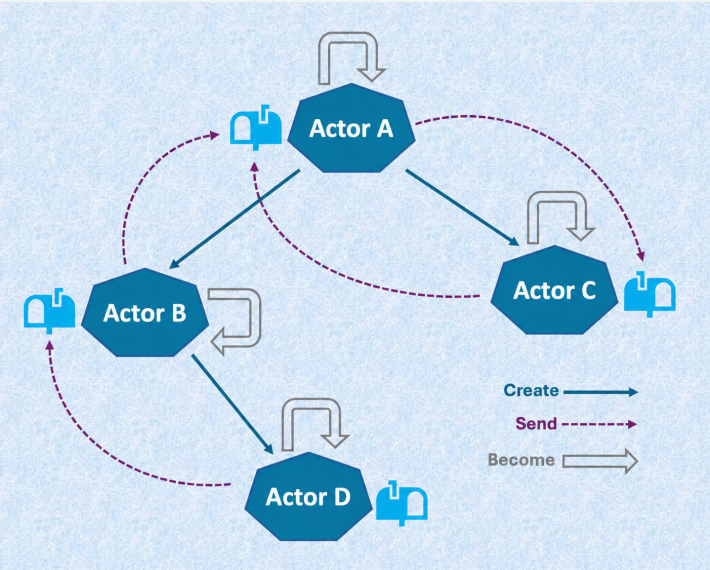

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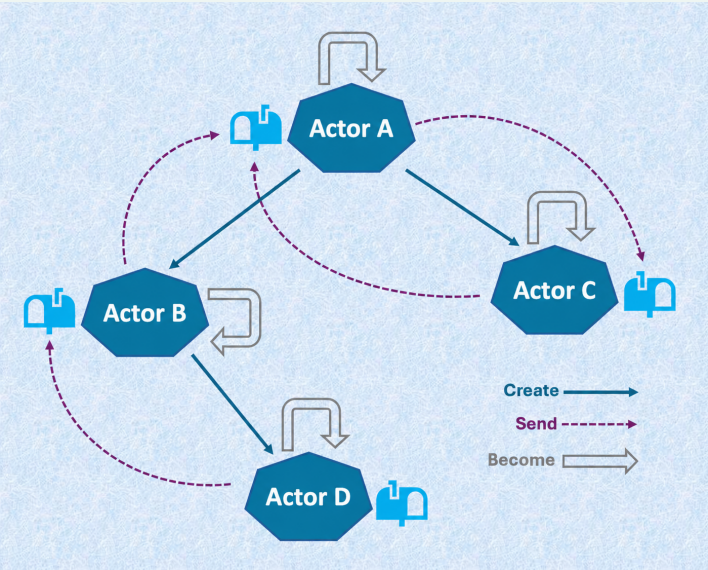

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Coordination by messages, not by global lockstep.

Why do actors fit?

The computation is naturally asynchronous.

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The computation is naturally asynchronous.

- each interval progresses at its own pace
- updated brackets communicated once discovered
- irrelevant work killed
- spare resources redirected immediately

Show me the money

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Move the human out of the critical path.

A parting wish

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Less babysitting. More discovery.