Hassle-Free Prediction of Excitation Wave Quenching using Actors

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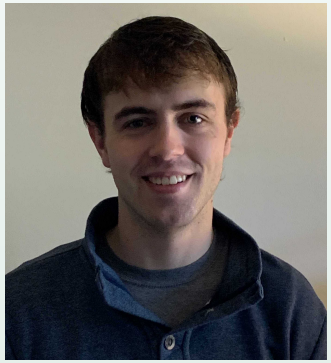
Acknowledgements

R. Spiteri



K. Klenk

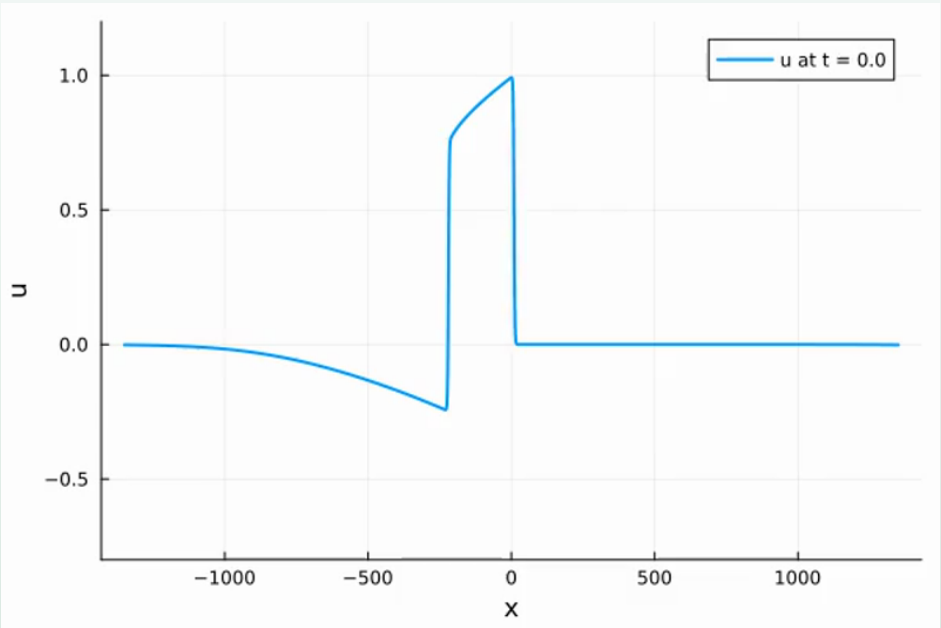
C. Marcotte

NSERC CRSNG

People. Discovery. Innovation.

Outline

Eliminate undesirable excitations

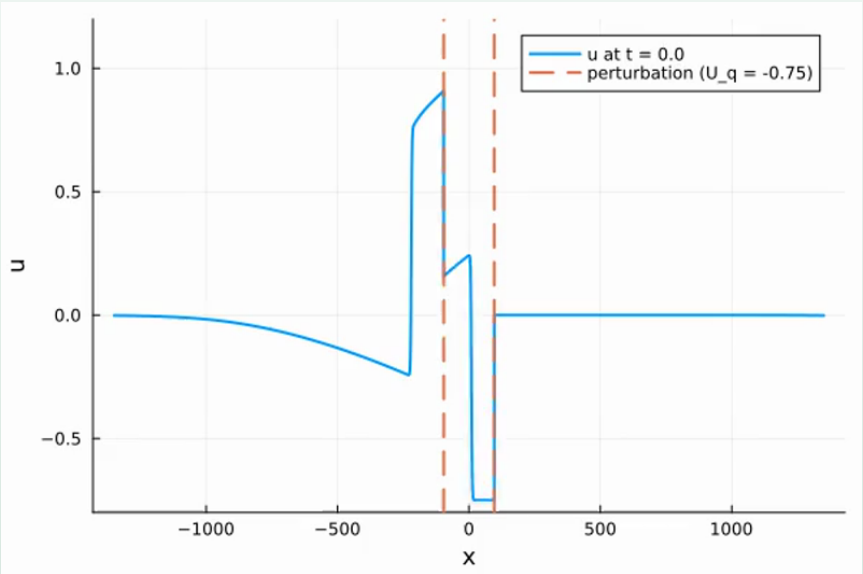


- Excitable media (e.g., nerve/cardiac tissue) support traveling waves
- Stable waves propagate indefinitely, but they can be quenched by perturbations

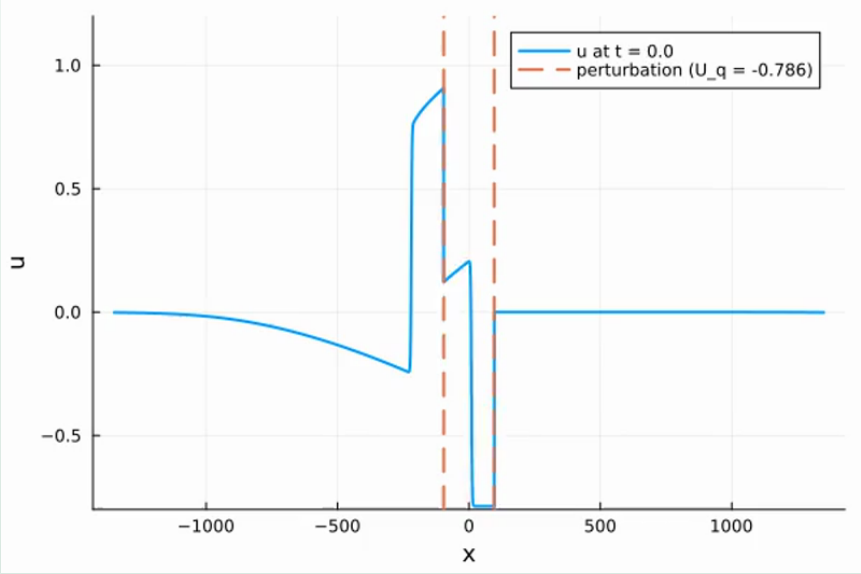
Marcotte, C. D. (2024), Predicting effective quenching of stable pulses in slow-fast excitable media, Physical Review E, 110(6), 064210.

Unquenched vs. Quenched

Unquenched wave

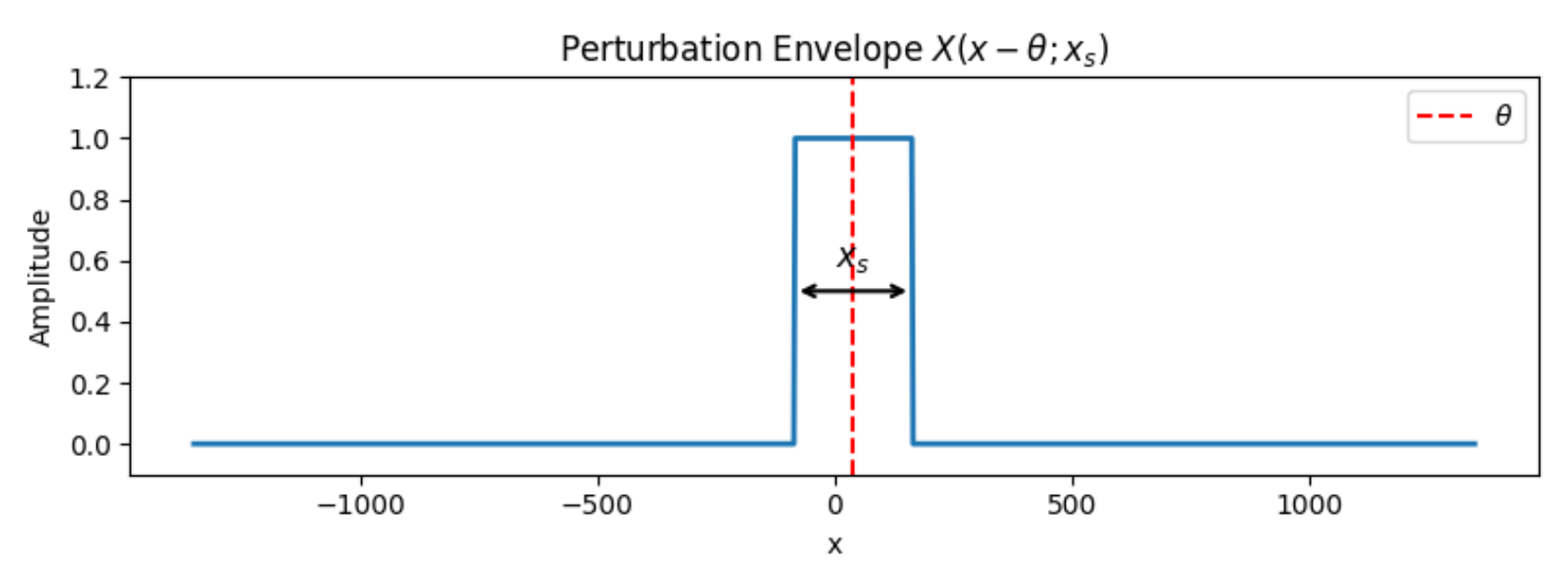


Quenched wave



Quenching threshold

- Smallest perturbation amplitude U_q^* that stops a wave
- Applied with pulse width x_s and at location θ



Computational Challenges

- Each quenching attempt needs a full PDE simulation
- Simulating as a large number of embarrassingly parallel jobs has drawbacks:
  - if number of cores $\not\approx$ number of jobs, must batch jobs
  - one job failure may result in loss of batch
  - batches subject to straggler effect

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We need faster, smarter strategies

FitzHugh–Nagumo Model

- Described by a system of reaction-diffusion PDEs:

$$\frac{\partial u}{\partial t} = D\nabla^2 u + u(u-\beta)(1-u) - w,$$
$$\frac{\partial w}{\partial t} = \gamma(\alpha u - w),$$

  - D is the diffusion coefficient
  - $u(x,t)$ is the excitation variable (fast)
  - $w(x,t)$ is the recovery variable (slow)
  - γ timescale separation
  - α, β are model parameters

Experimental Setup

- Domain : $x \in [0, L]$, where $L = 2700$, and $t \in [0, L/2\hat{c}]$ where $\hat{c}$ is the speed of the stable traveling pulse
- Initial conditions: A traveling excitation wave perturbed by an external stimulus given by

$$u(x, 0) = u_s(x) + U_q X(x - \theta; x_s),$$

  - $u_s(x)$ is a stable traveling wave solution
  - U_q is the perturbation amplitude
  - $X(x - \theta; x_s)$ is the perturbation envelope (localized pulse)

- Periodic boundary conditions

Experimental Setup Cont.

- $\gamma \in \{0.001, 0.01, 0.02, 0.025\}$
- $\theta \in [-40, 40]$ controls the center location of the perturbation
- $x_s \in [0, 700]$ controls the width (extent) of the perturbation
- We sample:

  θ every 5 units: $-40, -35, ..., 0, ..., 35, 40$

  x_s logarithmically between 0 and 700 (91 values)
- Total combinations: $4 \times 26 \times 91 = \mathbf{6}\ |\mathbf{188}$ jobs

How We Detect Quenching

- Define $\psi(T)$: deviation from rest

$$\psi(T) = \int_0^L |u(x,T) - \bar{u}|\, dx$$

- $\bar{u}$ is the value of u at rest

What Is the Unstable Wave?

- It's a special traveling wave that sits exactly at the boundary between:
  - A wave that recovers and keeps moving
  - A wave that collapses and returns to rest
- It's not stable: any tiny deviation makes it either grow or decay

Root-Finding for Threshold

- Solve:

$$F(U_q) = \psi(T; U_q, x_s, \theta) - \psi_{\text{unstable}} = 0$$

- ψ_{unstable} is the diagnostic value of the quenching metric $\psi(T)$ when the solution approaches the unstable traveling wave.
- Use Brent method to find U_q^*:
- Repeat for each (γ, x_s, θ) pair

Baseline Algorithm (Naïve)

For each parameter pair (γ, x_s, θ)**:**

1. Set an initial bracketing interval: $U_{q^{\min}}$, $U_{q^{\max}}$
2. Run a simulation with amplitude U_q
3. Check if wave quenched
4. Use root finder to refine U_q
5. Repeat until $|F(U_q)| < \varepsilon$

Actor Model

```cpp
#include "caf/all.hpp"


caf::behavior goodbye(caf::event_based_actor* self) {
  return {
    [=](const std::string& name) {
       self->println("Goodbye, " + name + "!");
      self->quit();
    }
  };
}

struct hello_state {
  int greet_count = 0;
};

caf::behavior hello(caf::stateful_actor<hello_state>* self) {
  return {
    [=](const std::string& name) {
      ++self->state().greet_count;
      self->println("Hello, " + name + "! Count: " + std::to_string(self->state().greet_count));
      self->become(goodbye(self));
    }
  };
}

void caf_main(caf::actor_system& system) {
    caf::scoped_actor self{system};
    auto hello_actor = system.spawn(hello);
    caf::anon_mail("World").send(hello_actor);
    caf::anon_mail("Alice").send(hello_actor);

    auto goodbye_actor = system.spawn(goodbye);
    caf::anon_mail("Bob").send(goodbye_actor);
}

CAF_MAIN()
```

→ Private state

→ Become

→ Create

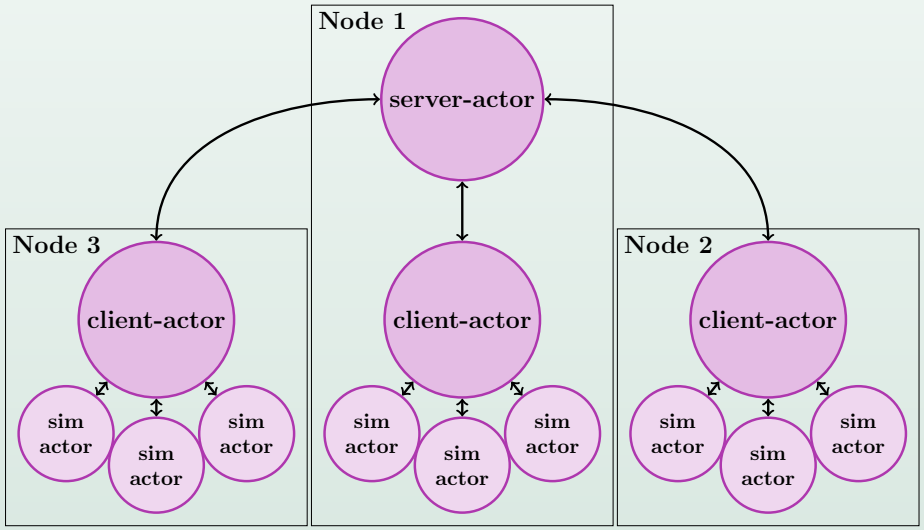
→ Communication through message

Output

```
Goodbye, Bob!
Hello, World! Count: 1
Goodbye, Alice!
```

Quenching-Actors

- **Server**: Generates jobs, manages progress
- **Client**: Spawns actors on remote nodes
- **Simulation**: Runs simulation, sends result



Smarter Bracketing Strategies

- Goal: Accelerate convergence to the quenching threshold U_q^*
- Use previously computed values to set tighter bracketing intervals:

  Same (γ, θ), nearby x_s: scale known U_q^* based on x_s
  Same (γ, x_s), smaller $|\theta|$: use U_q^* from more central positions
  Same (θ, x_s), larger γ: use U_q^* from faster waves

- Helps reduce failed root searches and shortens simulation time

Improved Algorithm (Actor-Based)

For each job (γ, θ, x_s)**:**

1. **[Server]** At first initializes job list and send jobs to client
   If there are some information in the cache, update the job list based on:

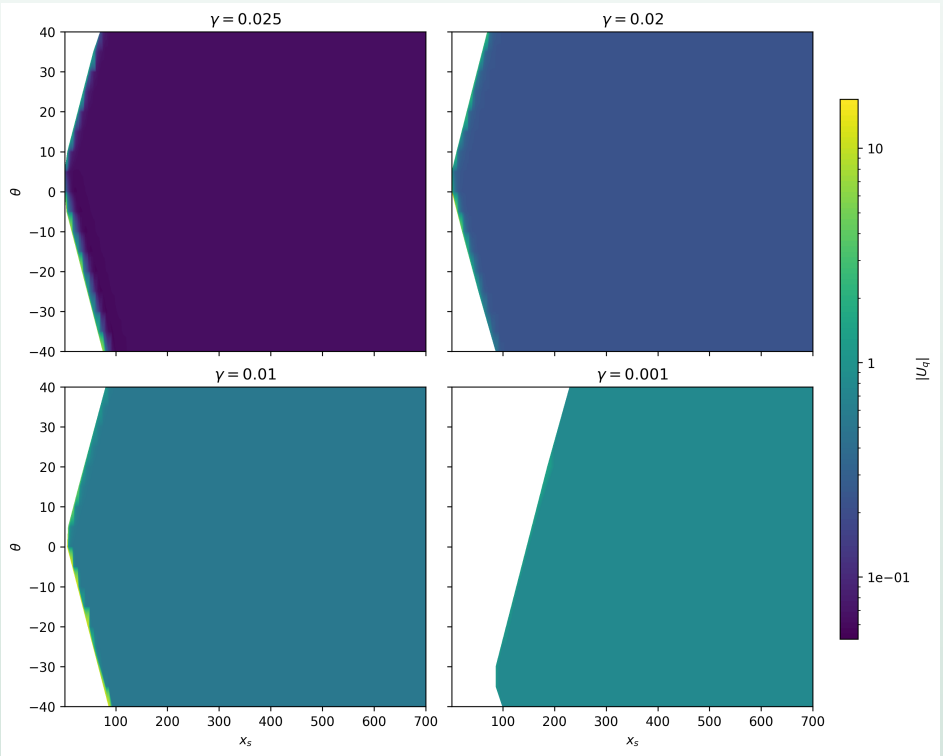
   Nearby x_s with same (γ, θ)
   Same (γ, x_s), smaller $|\theta|$
   Same (θ, x_s), larger γ

2. **[Client]** spawns actors on remote nodes
3. **[Client]** sends job to available worker
4. **[Worker]** receives a job
5. Set bracketing interval $[U_{q^{\min}}, U_{q^{\max}}]$ based on one
6. Run the solver with and send back the results
7. Save result in cache (`Uq_cache`(γ, θ))

Additional Details

- Space: 6th-order centered finite difference
- Time: BDF (`CVODE_BDF`) + GMRES (Sundials)
- The `Plato` cluster
- 5 nodes used were dual-socket Intel Xeon Gold 6226R @ 2.90GHz (Cascade Lake) processors (we used 30 cores on each node) connected to shared file system with EDR Infiniband
- More details: `https://wiki.usask.ca/display/ARC/Plato+HPC+Cluster`

Performance



- 6 188 simulations in sequence would take more than **100 days**
- Quenching-Actors without updating the brackets took **22:13:50** with 150 cores
- The CPU usage was **95.11%**

Performance Cont.

- Quenching-Actors with updating the brackets took **21:50:14** with 150 cores!
- It did not accelerate the simulation time significantly!
- Why?

Performance Cont.

- Quenching-Actors with updating the brackets took **21:50:14** with 150 cores!
- It did not accelerate the simulation time significantly!
- Why?
- The number of jobs that failed to find a quenching threshold was **3 358**!

Solution: Smolyak Sampling Instead of Exhaustive Sweeps

- **Problem:** Exhaustive sampling over (x_s, θ) is expensive, especially in regions where quenching is unlikely.
- **Observation:** Jobs that without quenching are both the slowest and the least informative.
- **Idea:** Use **Smolyak sampling** to adaptively select points that provide maximum information while reducing redundancy.

Smolyak Sampling: A Smarter Strategy (but not today)

- Smolyak sampling offers:
  - Sparse, adaptive exploration of parameter space
  - Focus near the quenching boundary
  - Fewer wasted simulations
- Do I have results yet? No!
- Will I have them next week? Probably!

Stay tuned for the sequel!

Conclusions

- The actor-based system enabled efficient parallel execution of wave quenching simulations
- Dynamic management of actors allowed for adaptive resource allocation and reduction in the burden on the user to fine-tune the simulation parameters