

# Parallel computation of fixed points on networks of nonlinear ODE

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## Motivation

- Networked dynamics describe various phenomena ranging from Michaelis-Menten gene regulation [4] to epidemic spreading processes [3].
- As networks become larger, our ability to simulate their dynamics is dependent on our ability to compute those dynamics in parallel.
- Parallel methods for numerical integration either require known finite time intervals, or excessive message passing, making parallel computation of asymptotic fixed points unrealistic to compute.

## The system

We consider dynamics on a graph  $G = (V, E)$  with adjacency matrix  $A$ . The derivative of each node  $x_i$  is given by the following sum [1].

$$\dot{x}_i = f(x_i) + \sum_{j=0}^{n-1} A_{ij}g(x_i, x_j) \quad (1)$$

$f(x_i)$  captures the intrinsic dynamics of each node arising from its current state.  $g(x_i, x_j)$  captures the extrinsic dynamics contributed from neighboring nodes. We specifically consider the following two systems which we refer to as regulatory dynamics and epidemic dynamics respectively.

$$\dot{x}_k = -Bx_k^f + \sum_j A_{kj}R \frac{x_k^h}{x_k^h + 1} \quad (2)$$

$$\dot{x}_k = -Bx_k + \sum_j A_{kj}R(1 - x_k)x_j \quad (3)$$

Here  $R$  and  $B$  are constants that change with the problem. We take them to be unit for our simulations.

## Dataset

Table 1: Networks taken from the Koblenz network repository that were used in experiments. The number of nodes and edges are displayed.

Network	Nodes	Edges
CA roads	1,965,206	2,766,607
PA roads	1,088,092	1,541,898
TX roads	1,379,917	1,921,660
Orkut	3,072,441	117,184,899
Livejournal	4,847,571	68,475,391
Google	875,713	5,105,039

## Timing

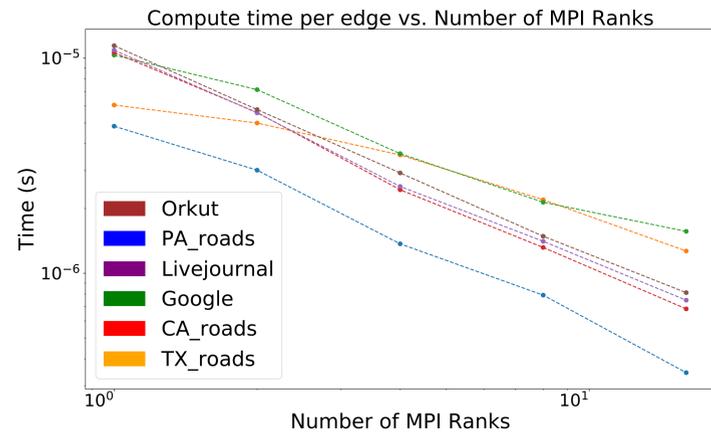


Figure 1: Compute times per edge for networks from Koblenz. These trials were done in 1,2,4,8, and 16 compute ranks. We see clear power law scaling.

## Accuracy

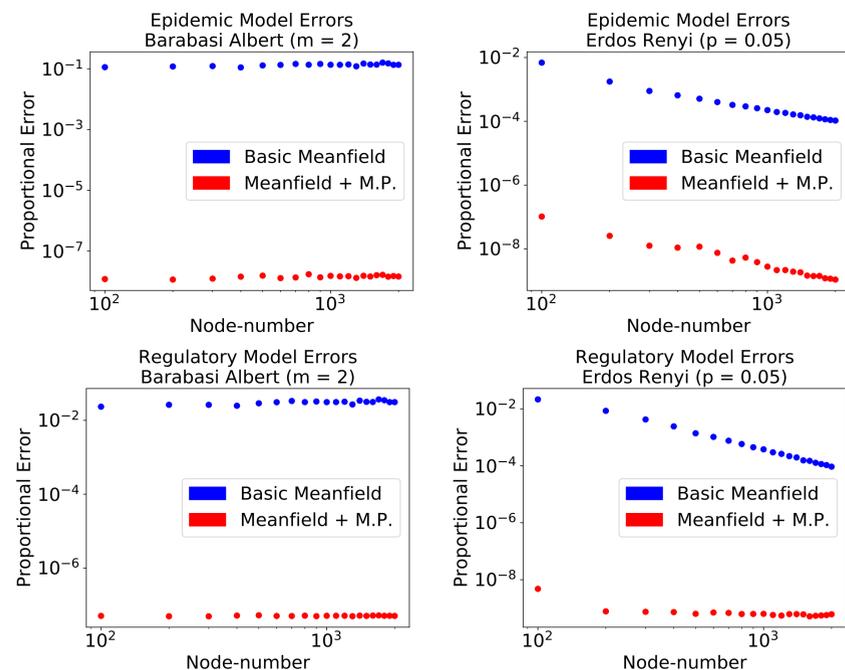


Figure 2: Error results for a suite of Barabási Albert and Erdős Rényi networks for the regulatory dynamics 2 and epidemic dynamics 3. We see clear differences in accuracy for both the differing dynamics and differing topologies.

## Method

- Observation:** If a network has steady state  $\mathbf{x}^*$ , a subnetwork will evolve towards that steady state if the state of each exterior neighboring node  $v_i$  is held constant at  $x_i^*$ .
- We perform a series of meanfield approximations as in [2] to obtain the following equation where  $\beta$  is the network resilience.

$$\dot{x} = f(x) + \beta g(x, x) \quad (4)$$

- We calculate the fixed point of this one-dimensional equation  $x_{eff}$ .
- We then partition the network amongst our compute ranks and numerically integrate each rank using  $x_{eff}$  as a stand in for the true dynamics outside of our subnetwork to obtain steady state  $x^*(0)$ .
- Then calculate the proportional error as  $\epsilon = \frac{\|x_0^* - x^*\|}{\|x^*\|}$ .
- To improve this error we can exchange information between ranks and then numerically integrate again using the initial steady state estimate  $x^*(0)$  as a stand in for the dynamics exterior to our subnetwork. This yields a second estimate  $x^*(1)$ .
- This can then be iterated to improve accuracy further.

## Findings

- As expected from [2] the proportional error of  $x^*(0)$  diminishes as the network topology becomes more regular.
- We find that additional message passing drastically improves accuracy of later estimates  $x^*(k)$ .
- We also find that the wall time scales well with the number of processors and that the per-edge computation time is similar across varying network topologies.

## References

- Gao J.; Barzel; and Barabási. Universal resilience patterns in complex networks. *Nature*, 530(7590):307, 2016.
- Jiang C.; Gao; Magdon-Ismail. True nonlinear dynamics from incomplete networks. *arXiv:2001.06722v1*, 2020.
- Pastor-Satorras R. and A. Vespignani. Epidemic spreading in scale-free networks. *Rhys. Rev. Lett.*, 86(14):3200, 2001.
- Alon U. An introduction to systems biology: design principles of biological circuits. *Chapman and Hall/CRC*, 2006.