Large-scale optimization-based non-negative computational framework for diffusion equations: parallel implementation and performance studies

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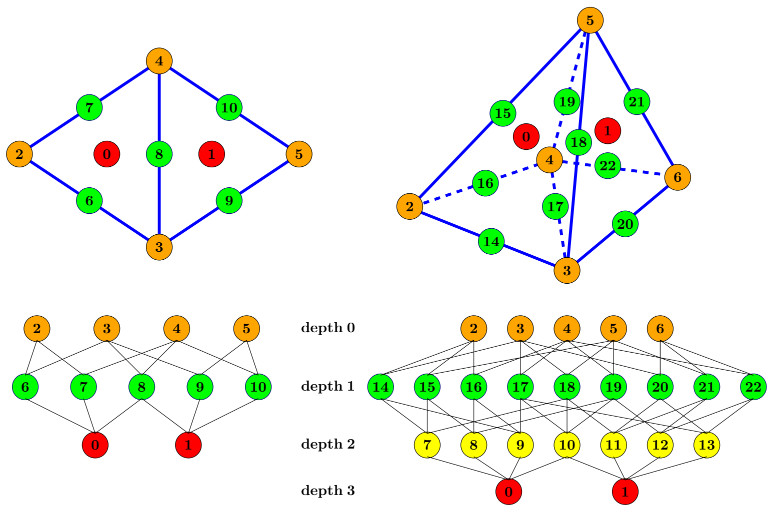
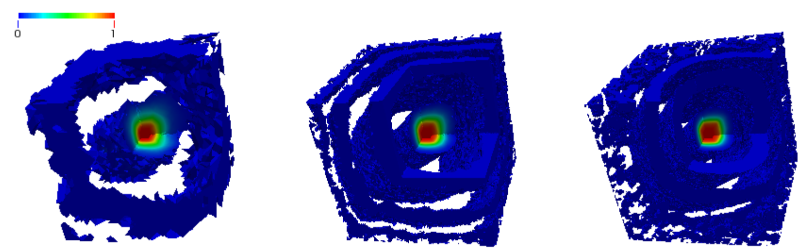
PETSc Conference and Workshop
June 15th – 18th, 2015

Introduction and Motivation

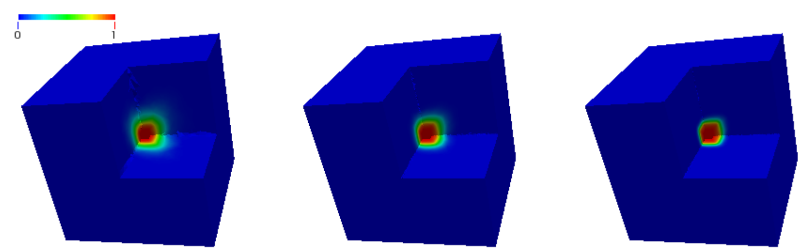
- The Galerkin Finite Element Method does not satisfy the discrete maximum principles for anisotropic diffusion
- Recent studies have proposed **convex optimization** techniques to overcome this setback
- So far these have only been tested on small and 2D academic problems



Mesh representation has a Hasse Diagram



Galerkin solution (with negative concentrations)

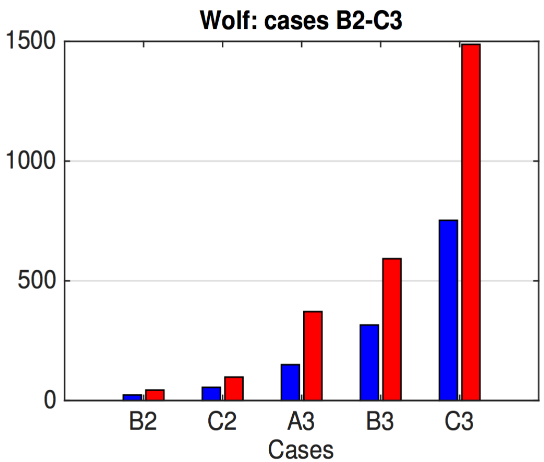


Non-negative methodology

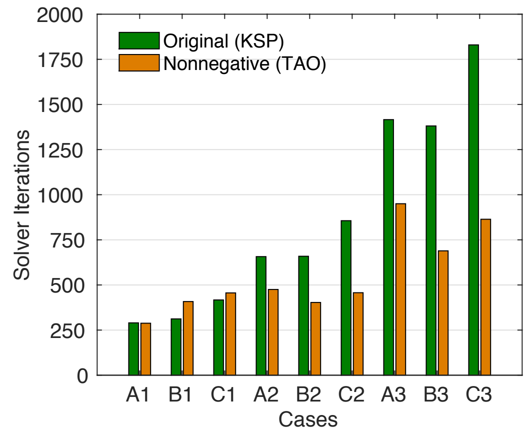
Aim of this work:

1. Solve anisotropic diffusion leveraging PETSc's TAO and DMPlex features
2. Ensures non-negative solutions for larger and more realistic problems
3. Document the performance metrics

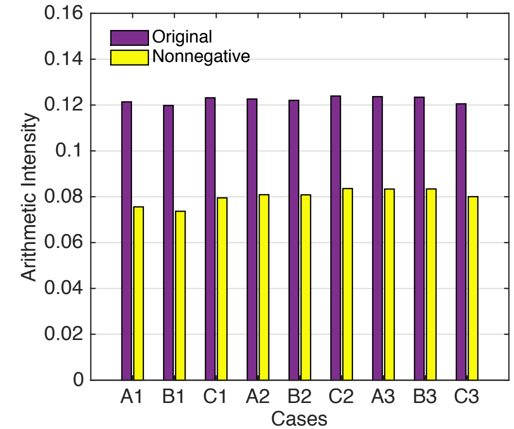
Performance studies



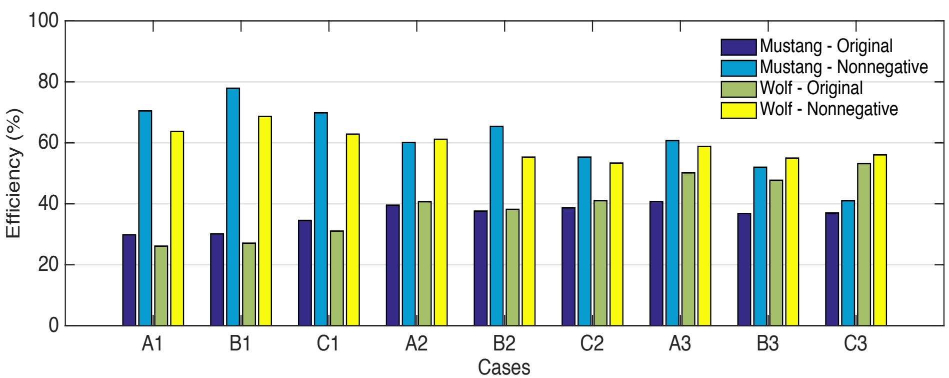
Wall-clock time (s)



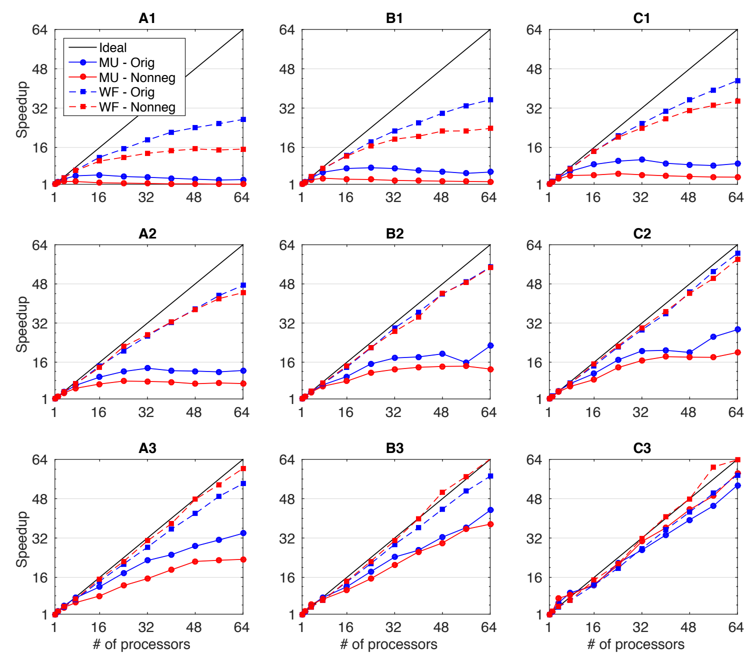
Solver iterations



Arithmetic Intensity



Efficiency based on the Roofline model



Speedup

Chromium contamination