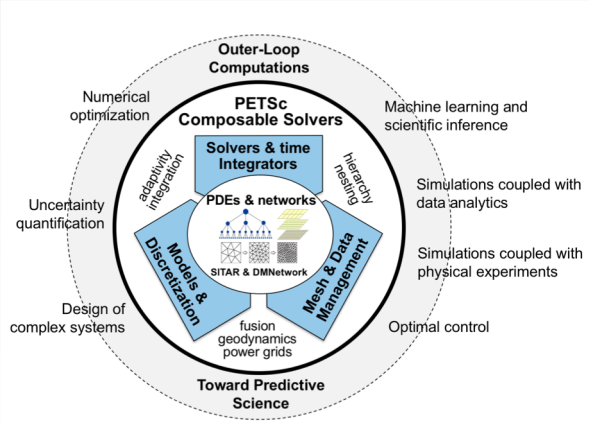
Scalable Network PDE-Based Multiphysics Simulation using the PETSc Library

Hong Zhang, Getnet Betrie, Barry Smith, and PETSc Team
Argonne National Laboratory

PETSc:

Portable Extensible Toolkit for Scientific Computations

https://www.mcs.anl.gov/petsc



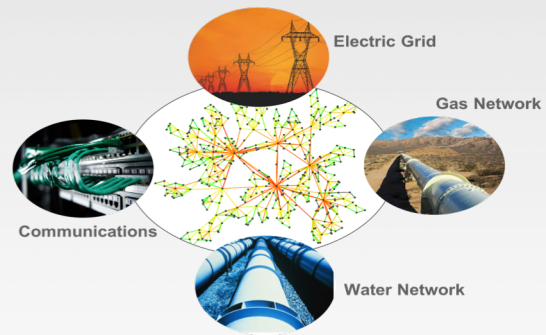
DMNetwork:

Multiphysics PDE-based network simulations, integrating composable solvers and topology management.

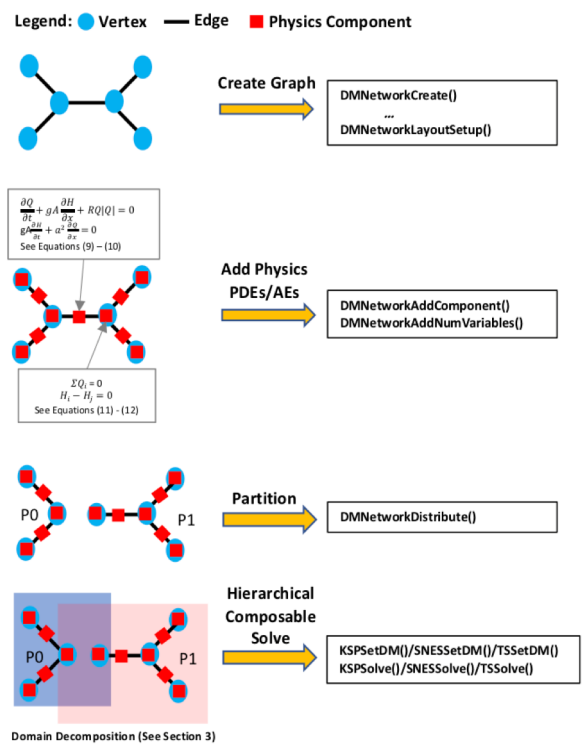
Potential Impact

- Efficiency and flexibility simultaneously
- Multiphysics simulations at scale
- Interdisciplinary dialogue by utilizing unified data abstractions

Applications



DMNetwork Application Steps



Experiments

Water pipe network:

$$\frac{\partial Q^k}{\partial t} + gA\frac{\partial H^k}{\partial x} + RQ^k\left|Q^k\right| = 0,$$
$$gA\frac{\partial H^k}{\partial t} + a^2\frac{\partial Q^k}{\partial x} = 0,$$

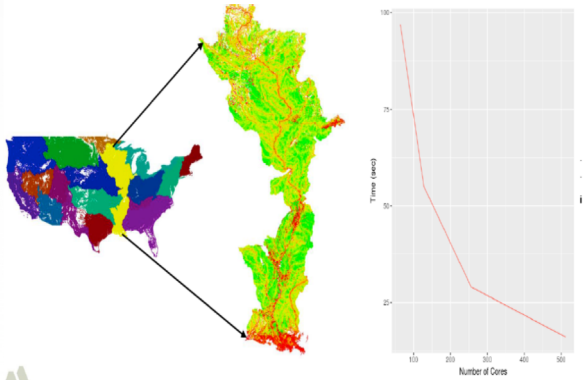
$$\sum_{j=1}^{ne_i} Q_i^{k_j} = 0,$$
$$H_i^{k_j} - H_i^{k_1} = 0, \quad j = 2 \ldots ne_i.$$

Table IV. Execution Time of Transient State on Edison

No. of Cores	Variables (in millions)	Maximum Variables per Core (in thousands)	Linear Preconditioner: Block Jacobi	ASM ov. 1	ASM ov. 2
240	16	106	9.9 (48)	7.3 (25)	6.4 (20)
960	63	106	10.6 (55)	7.0 (24)	6.2 (20)
3,840	253	106	10.4 (53)	7.3 (24)	6.7 (20)
15,360	1,012	104	11.9 (53)	11.4 (26)	9.9 (20)
30,720	2,023	117	20.0 (53)	17.6 (26)	17.2 (20)

River network:

- The Mississippi River with 263,531 river networks and 28,894,804 unknowns simulated on Theta
- The river represents 1/8th of the total river networks in the conterminous U.S.
- The scaling results show doubling the number of cores from 64 to 512 reduced the computation time from 96 to 12 seconds
- Future work is on progress to simulate the entire river networks in the conterminous U.S.



References

Scalable multiphysics network simulation using PETSc DMNetwork
DA Maldonado, S Abhyankar, B Smith, H Zhang - Argonne National Laboratory, 2017