Using AmgX to Accelerate PETSc-Based CFD Codes

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Our Group

- Professor Lorena A. Barba
  http://lorenabarba.com/
- Projects:
  - **PyGBe** - *Python GPU code for Boundary elements*
    https://github.com/barbagroup/pygbe
  - **PetIBM** - *A PETSc-based Immersed Boundary Method code*
    https://github.com/barbagroup/PetIBM
  - **cuIBM** - *A GPU-based Immersed Boundary Method code*
    https://github.com/barbagroup/cuIBM
  - *… and so on*
    https://github.com/barbagroup

Our story

How we accelerate PetIBM using AmgX.

PetIBM

Solving Poisson systems in CFD solvers is already tough, but ...

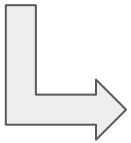
Solving modified Poisson systems is tougher

Taira & Colonius' method (2007):

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u} + \int_s \mathbf{f}(\boldsymbol{\xi}(s,t)) \delta(\boldsymbol{\xi} - \mathbf{x}) \, \mathrm{d}s,$$

$$\nabla \cdot \mathbf{u} = 0,$$

$$\mathbf{u}(\boldsymbol{\xi}(s,t)) = \int_{\mathbf{x}} \mathbf{u}(\mathbf{x}) \delta(\mathbf{x} - \boldsymbol{\xi}) \, \mathrm{d}\mathbf{x} = \mathbf{u}_B(\boldsymbol{\xi}(s,t)),$$



$$\begin{bmatrix} A & G & E^{\mathrm{T}} \\ G^{\mathrm{T}} & 0 & 0 \\ E & 0 & 0 \end{bmatrix} \begin{pmatrix} q^{n+1} \\ \phi \\ \tilde{f} \end{pmatrix} = \begin{pmatrix} r^n \\ 0 \\ u_B^{n+1} \end{pmatrix} + \begin{pmatrix} bc_1 \\ -bc_2 \\ 0 \end{pmatrix}$$

[†]K. Taira and T. Colonius, "The immersed boundary method: A projection approach", Journal of Computational Physics, vol. 225, no. 2, pp. 2118-2137, 2007.

Solving modified Poisson systems is tougher

$$Q \equiv [G,\ E^{\mathrm{T}}], \quad \lambda \equiv \begin{pmatrix} \phi \\ \tilde{f} \end{pmatrix}, \quad r_1 \equiv r^n + bc_1, \quad r_2 \equiv \begin{pmatrix} -bc_2 \\ u_B^{n+1} \end{pmatrix}$$

$$\begin{bmatrix} A & 0 \\ Q^{\mathrm{T}} & -Q^{\mathrm{T}}B^N Q \end{bmatrix} \begin{bmatrix} I & B^N Q \\ 0 & I \end{bmatrix} \begin{pmatrix} q^{n+1} \\ \lambda \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} + \begin{pmatrix} -\frac{\Delta t^N}{2^N}(LM^{-1})^N Q\lambda \\ 0 \end{pmatrix}$$

$$Aq^* = r_1 \qquad \text{(Solve for intermediate velocity)},$$

$$Q^{\mathrm{T}}B^N Q\lambda = Q^{\mathrm{T}}q^* - r_2 \qquad \text{(Solve the modified Poisson equation)},$$

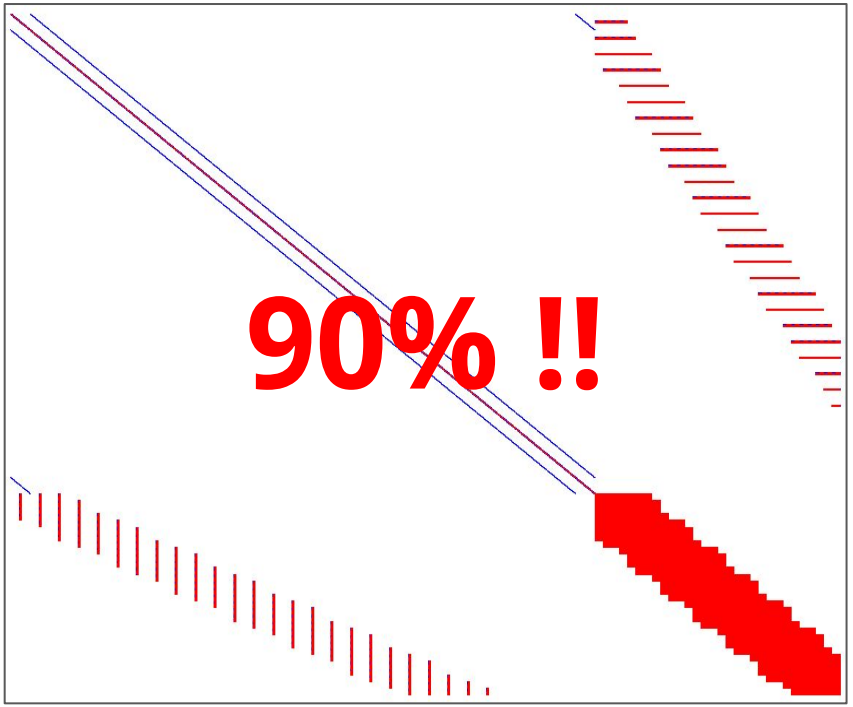
$$q^{n+1} = q^* - B^N Q\lambda \qquad \text{(Projection step)}.$$

Solving modified Poisson systems is tougher

Possible solutions:

Rewrite the whole program for multi-GPU capability, or

Tackle the expensive part !



AmgX and why AmgX?

AmgX

- **Krylov methods:**
  - CG, GMRES, BiCGStab, … etc
- **Multigrid preconditioners:**
  - Classical AMG (largely based on Hypre BoomerAMG)
  - Unsmoothed aggregation AMG
- **Smoothers:**
  - Block-Jacobi, Gauss-Seidel, incomplete LU, Polynomial, dense LU … etc
- **Cycles:**
  - V, W, F, CG, CGF

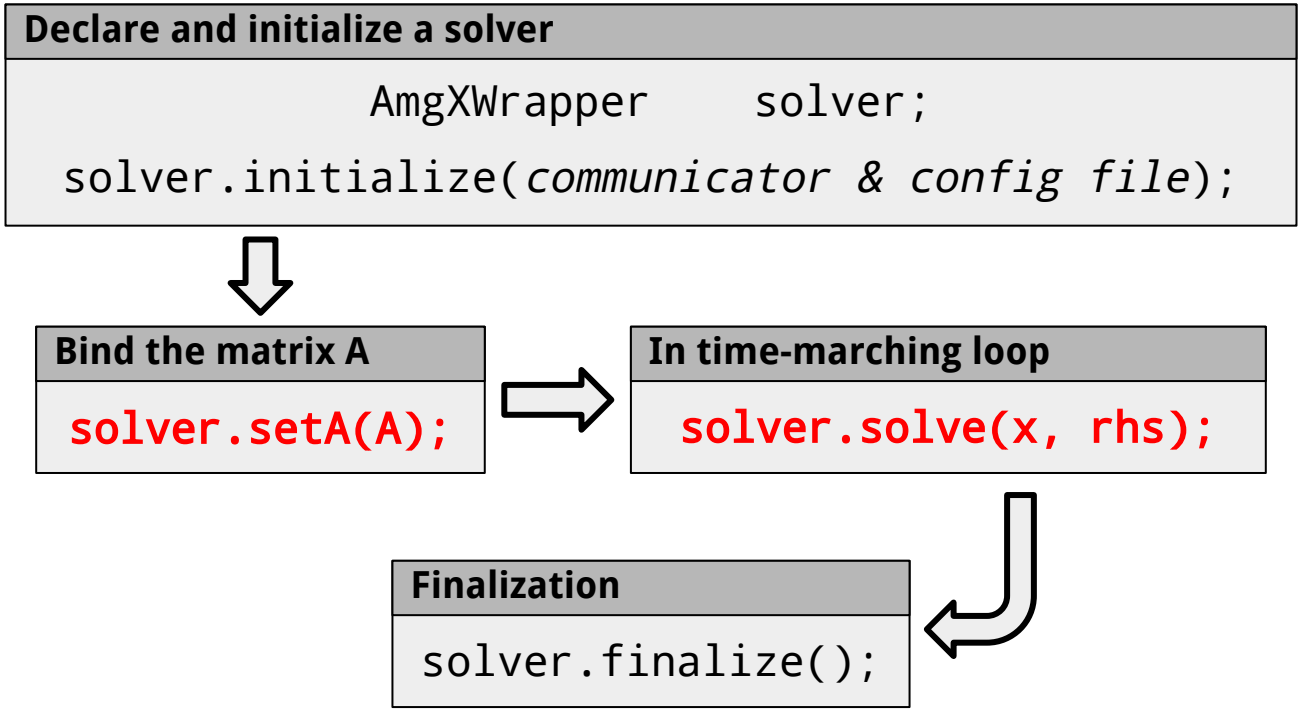
AmgX

- **Multiple GPUs on single node / multiple nodes:**
  - MPI (OpenMPI) / MPI Direct
  - Single MPI rank ⇔ single GPU
  - Multiple MPI ranks ⇔ single GPU
- **C API**
- **Unified Virtual Addressing**
- **Developed and supported by NVIDIA**
  - https://developer.nvidia.com/amgx

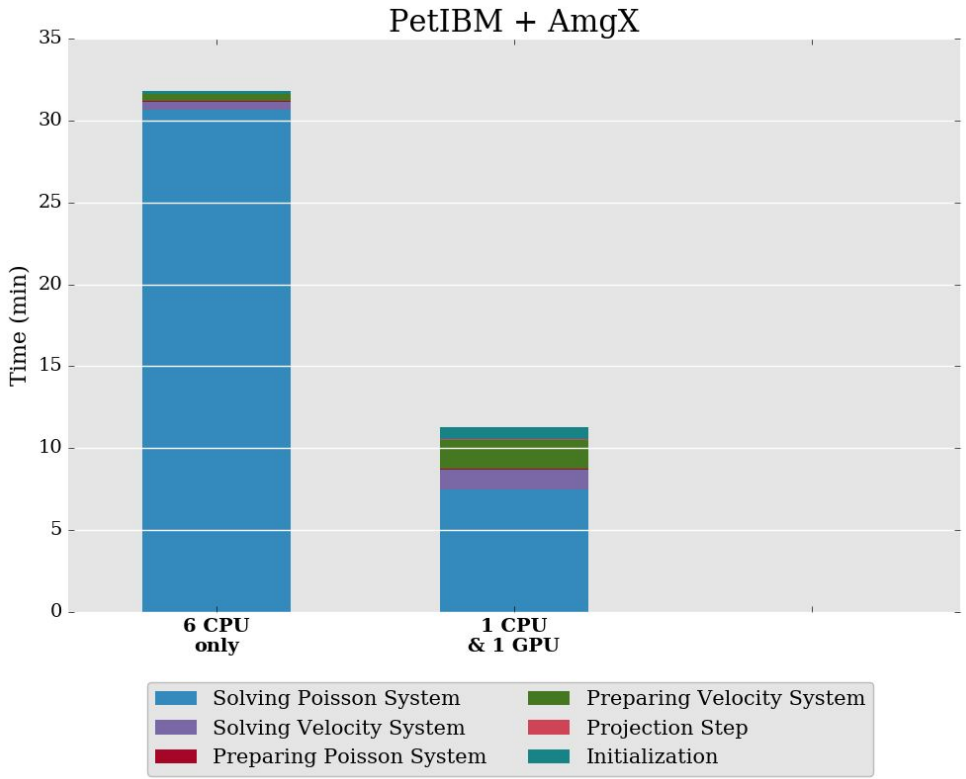
AmgX Wrapper

A wrapper for quickly coupling AmgX into existing PETSc-based software

AmgX Wrapper: Make Life Easier



Example: 2D Cylinder Flow, Re=40



- Mesh Size: 2.25M
- 1 NVIDIA K40c
- Velocity:
  - PETSc KSP - CG
  - Block Jacobi
- Modified Poisson
  - AmgX - CG
  - Aggregation AMG

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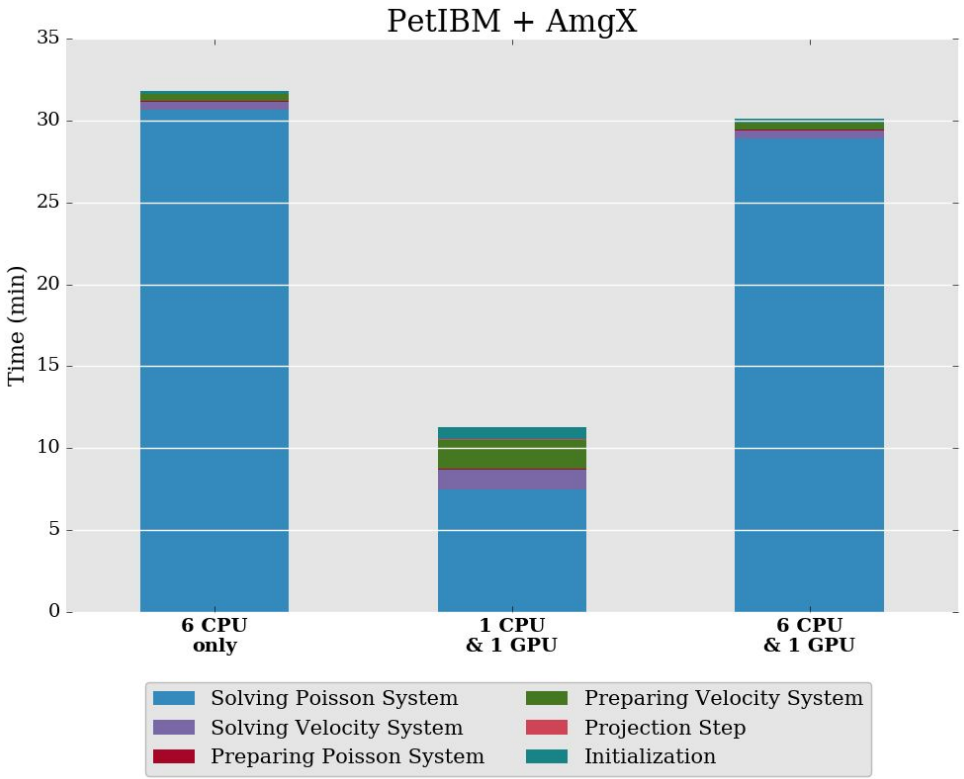

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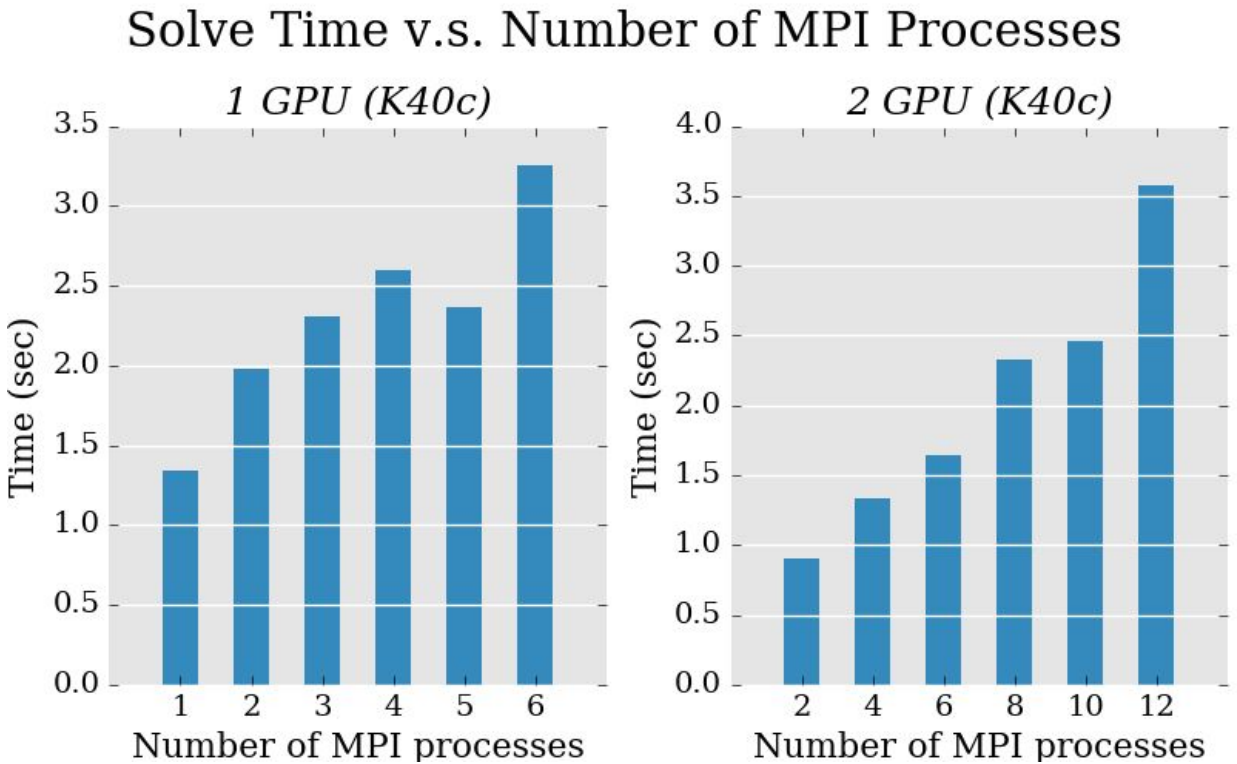
Issue

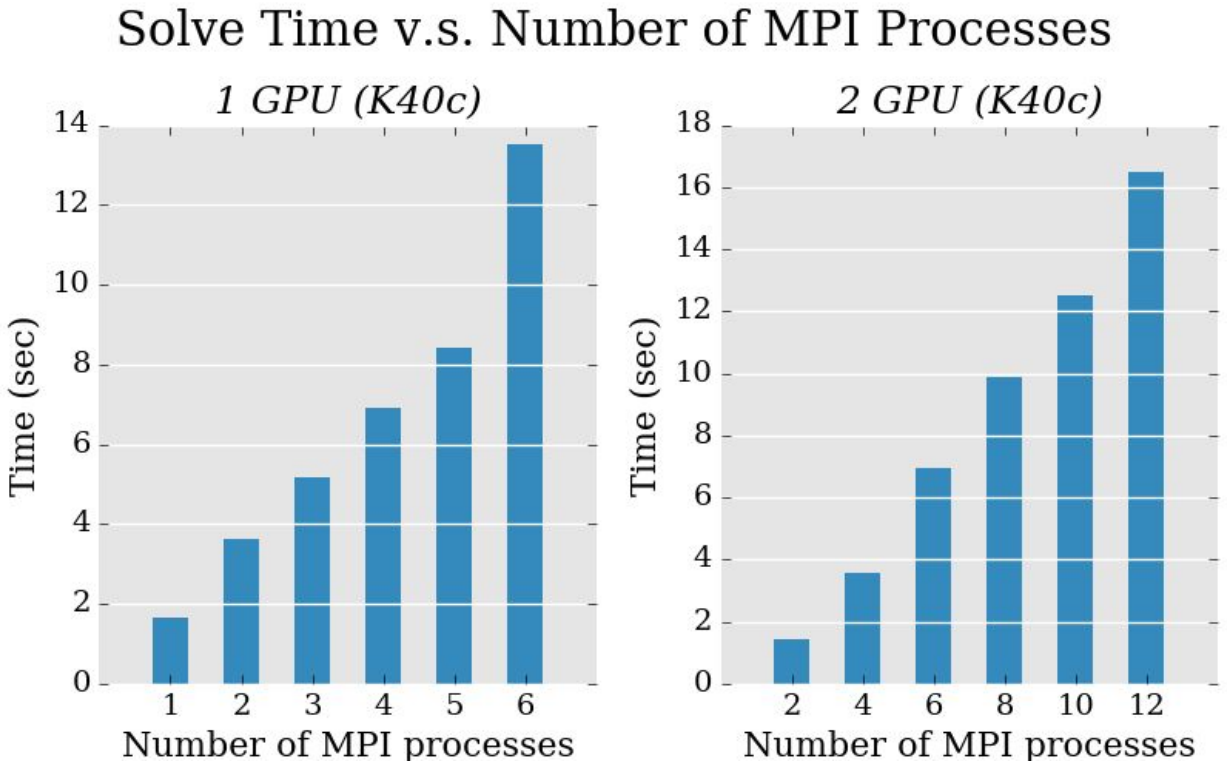
When we have more MPI ranks than GPUs

Tests: 3D Poisson



- 6M unknowns
- Solver:
  - CG
  - Classical AMG

Tests: Modified Poisson Equation

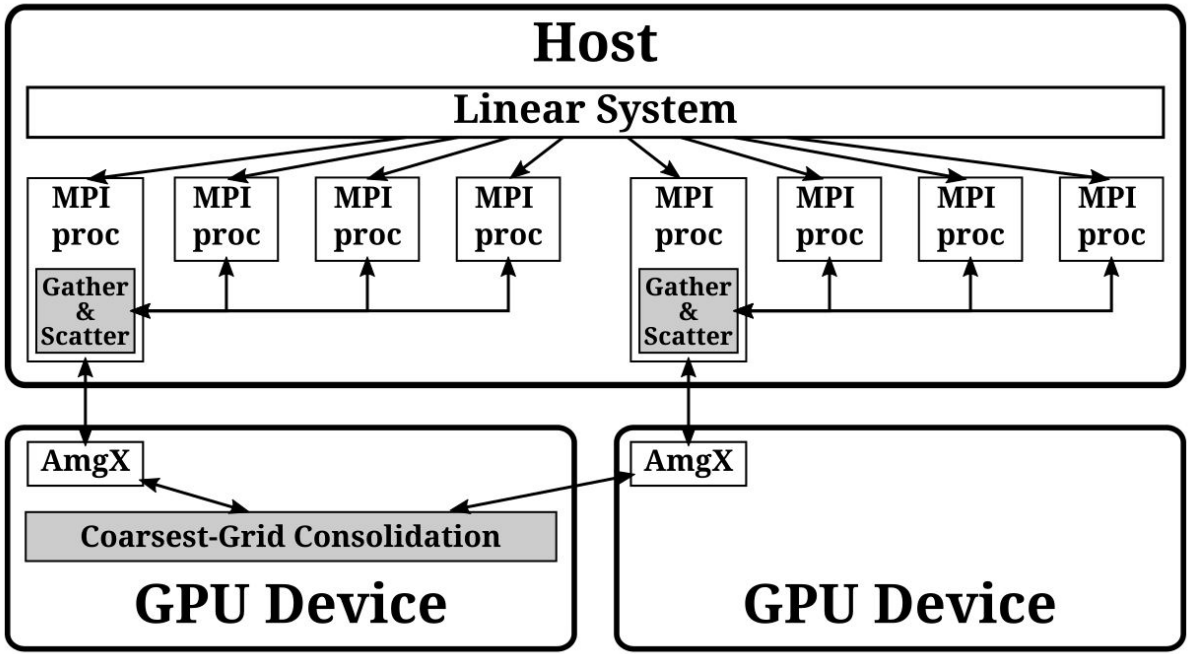


- 2D Cylinder, Re 40
- 2.25M unknowns
- Solver:
  - CG
  - Aggregation AMG

We want to make using AmgX easy

The wrapper makes things easier

No need to modify original codes in PETSc-based applications



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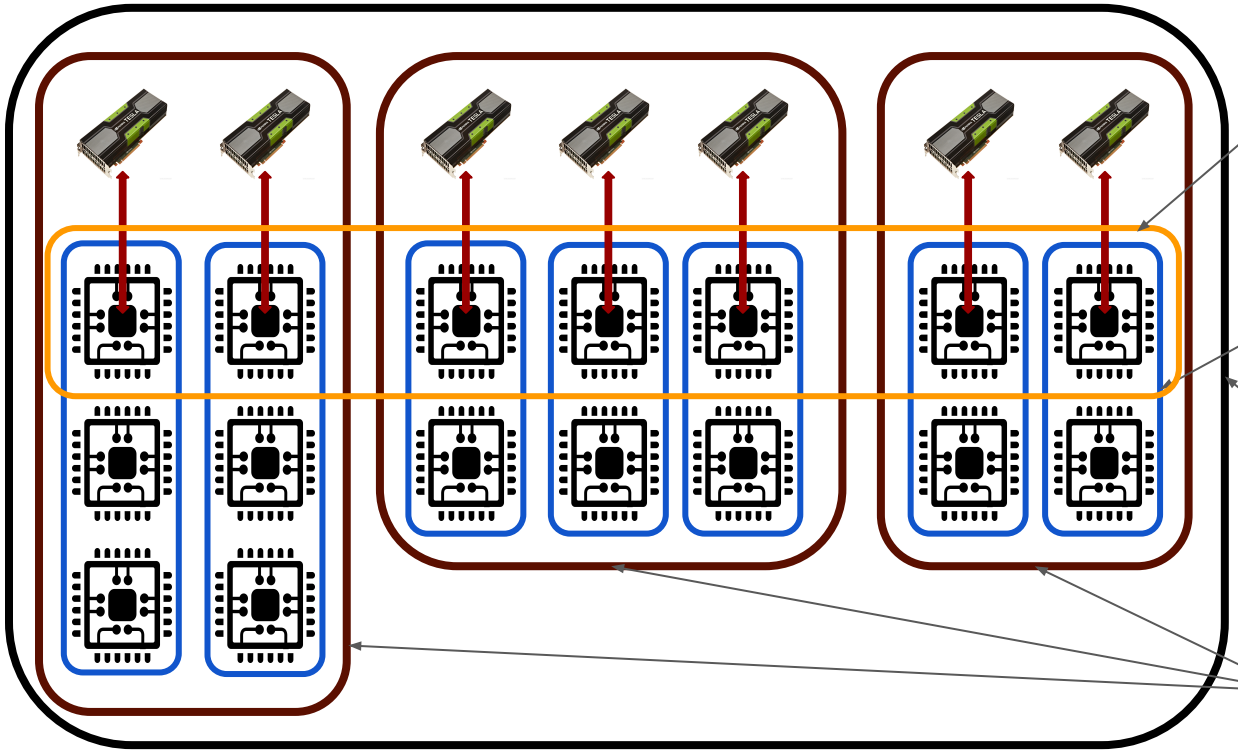


CPU ⇔ GPU Communicator

Matrix Consolidation Communicator

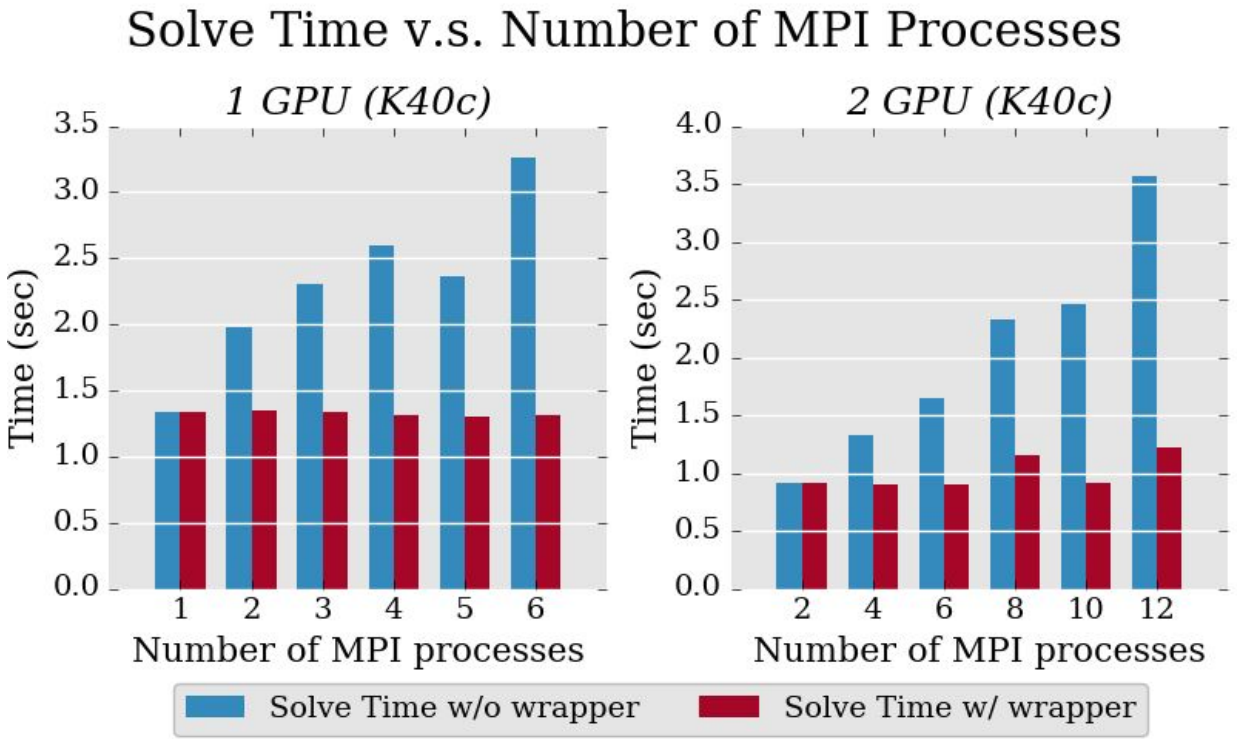
Global Communicator

In-Node Communicator

Does it work well?

Time spent on communication? Worth or not?

Check: 3D Poisson



- 6M unknowns
- Solver:
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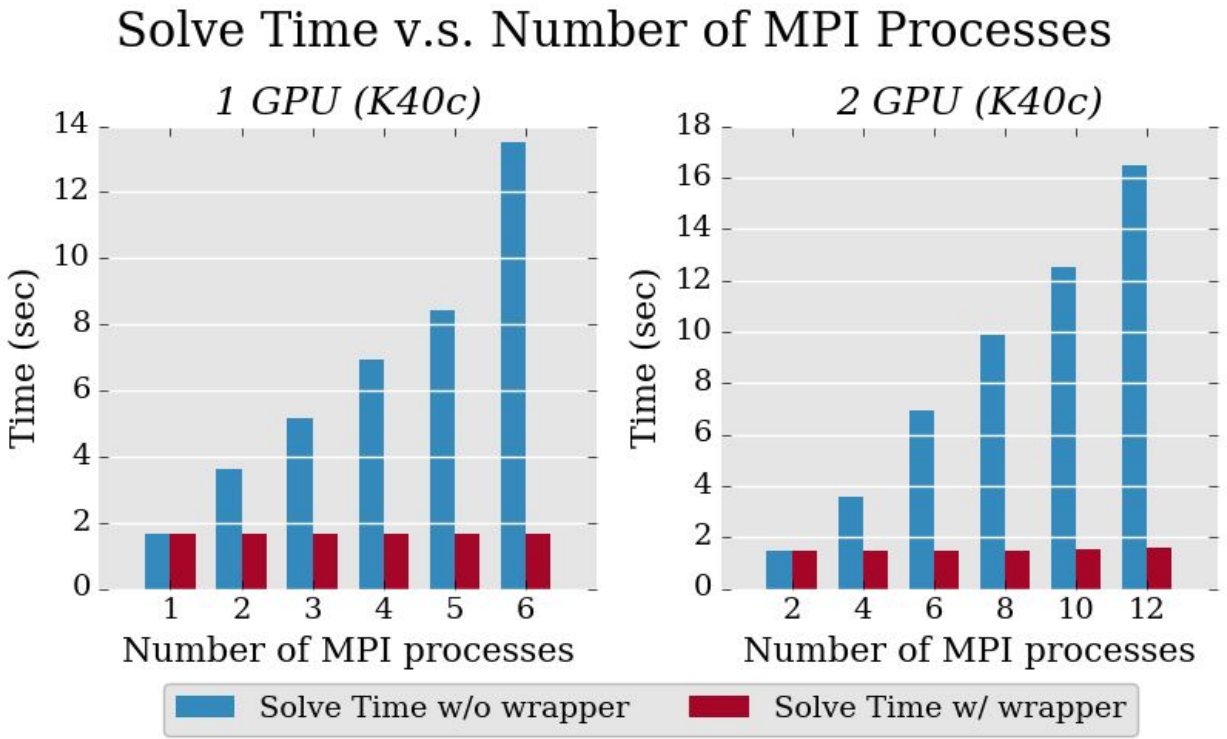
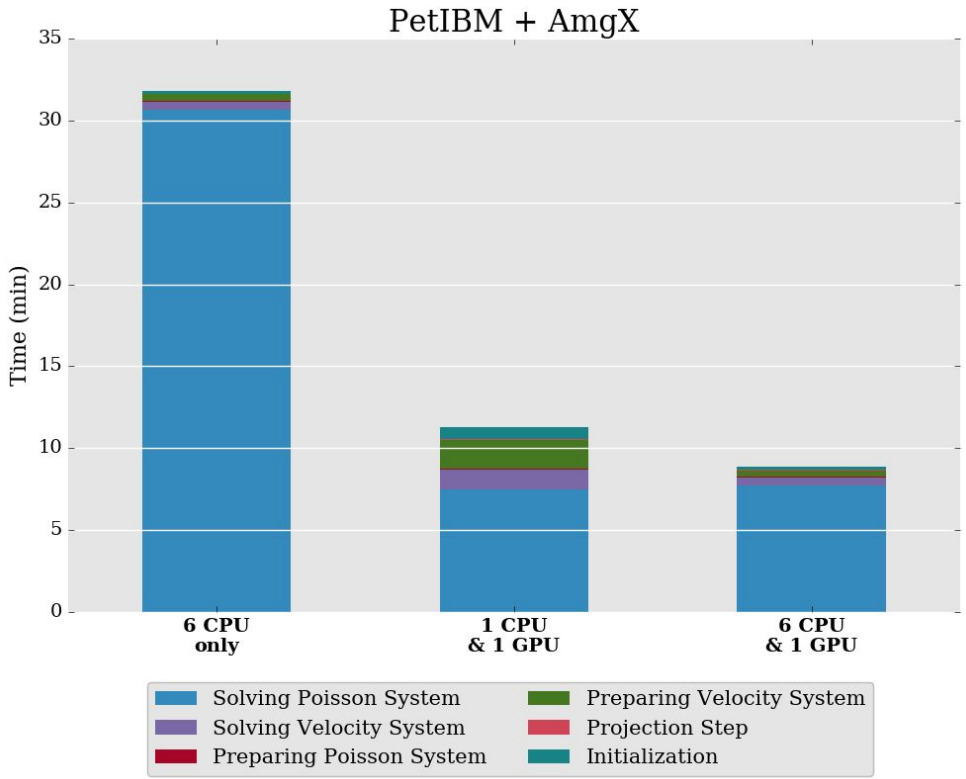
Check: Modified Poisson Equation



- 2D Cylinder, Re 40
- 2.25M unknowns
- Solver:
  - CG
  - Aggregation AMG

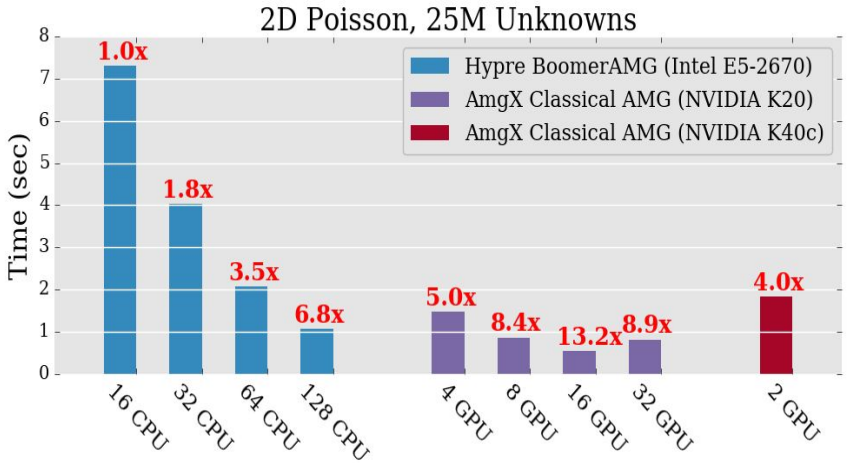
Back to Example: 2D Cylinder Flow, Re=40

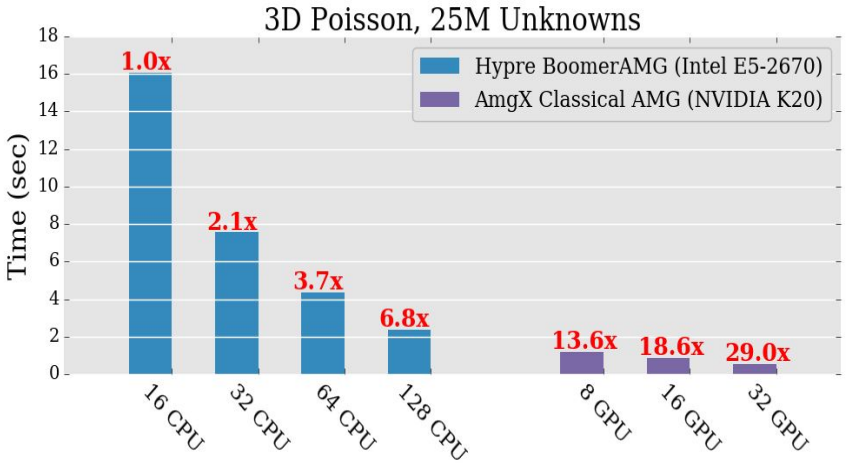


- Mesh Size: 2.25M
- 1 NVIDIA K40c
- Velocity:
  - PETSc KSP - CG
  - Block Jacobi
- Modified Poisson
  - AmgX - CG
  - Aggregation AMG
- AmgX Wrapper

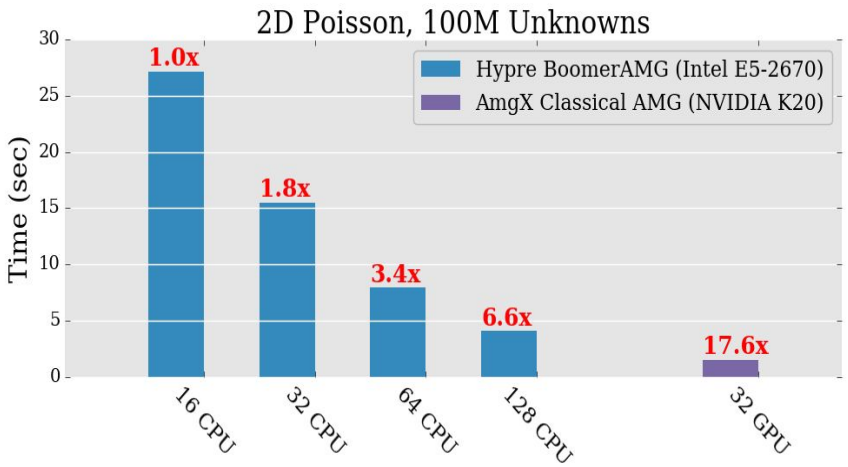
Tests and benchmarks

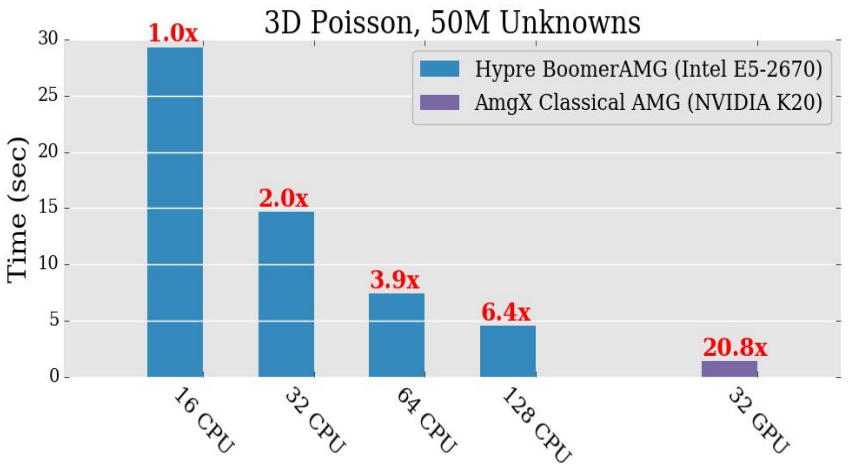
Example: Medium-Size Problems



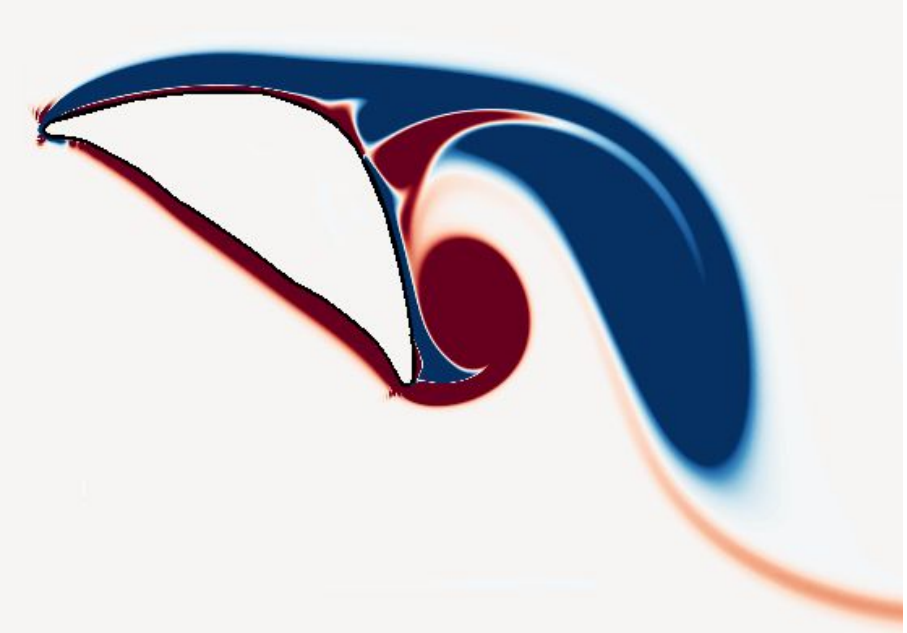


Example: Large-Size Problems





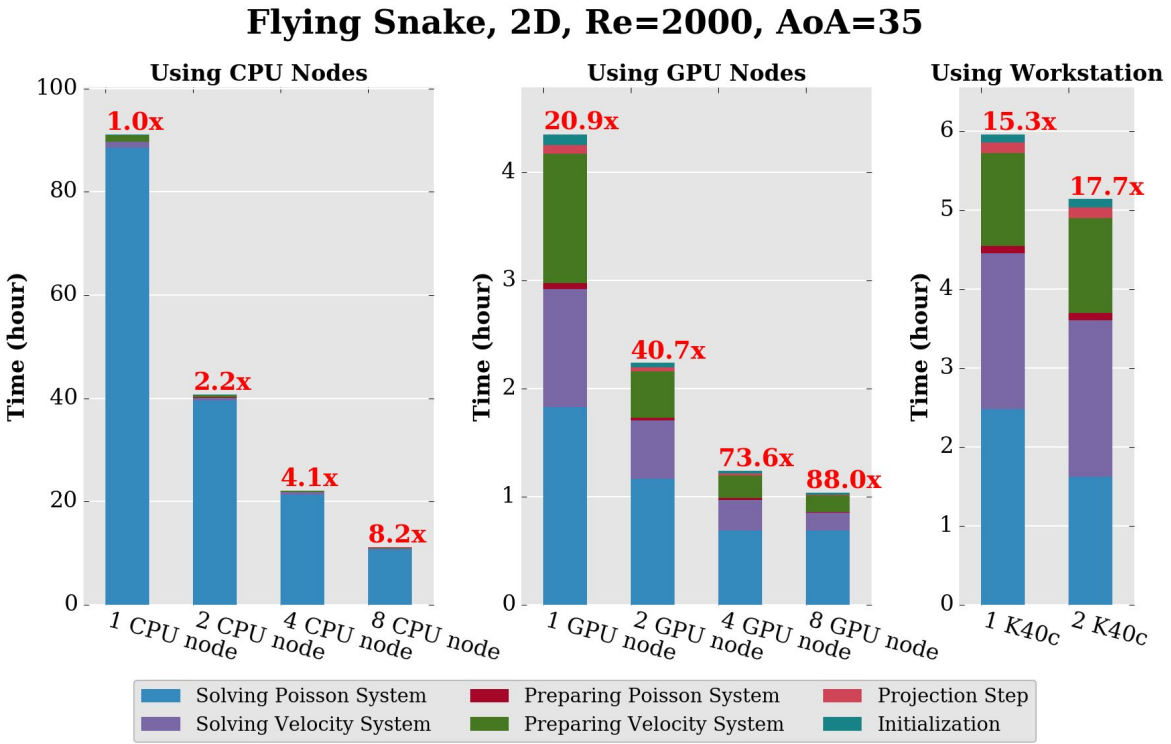
Example: Flying Snakes



- **Anush Krishnan et. al. (2014)[†]**
  - **Re=2000**
  - **AoA=35**
  - **Mesh Size: 2.9M**

[†]A. Krishnan, J. Socha, P. Vlachos and L. Barba, "Lift and wakes of flying snakes", *Physics of Fluids*, vol. 26, no. 3, p. 031901, 2014.

Example: Flying Snakes



- **Per CPU node:**
  - 2 Intel E5-2620 (12 cores)
- **Per GPU node:**
  - 1 CPU node (12 cores)
  - 2 NVIDIA K20
- **Workstation:**
  - Intel i7-5930K (6 cores)
  - 1 or 2 K40c

Time is money

Potential saving on hardware

Adding GPUs to existing workstations or the existing computing nodes has more benefits than adding more computing nodes does

Potential Savings and Benefits: Hardware

To achieve the same speed up, GPUs may be a better choice than CPUs. It reduces:

- costs on extra hardware,
    - motherboards, memory, hard drives, cooling systems, power supplies, Infiniband switches, physical space… etc.
- works and human resources on managing clusters,
- socket to socket communications
- potential runtime crash due to single node failure or network failure, and
- time spent on queue at any HPC centers

Potential saving on cloud HPC service

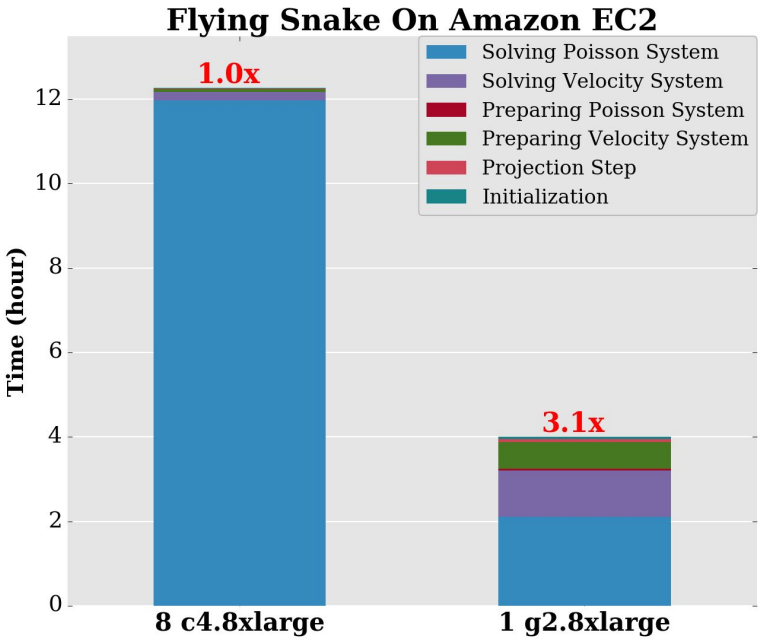
Running GPU-enabled CFD applications with cloud HPC service may save a lot

Potential Saving and Benefits: Cloud HPC Service

Reduce execution time and needed nodes. For example, on Amazon EC2:

- **GPU nodes - g2.8xlarge:**
  - 32 vCPU (Intel E5-2670) + 4 GPUs (Kepler GK104)
  - Official Price: $2.6 / hr
  - Possible Lower Price (Spot Instances): < $0.75 / hr
- **CPU nodes - c4.8xlarge**
  - 36 vCPU (Intel E5-2663)
  - Official Price: $1.675 / hr
  - Possible Lower Price (Spot Instances): < $0.6 / hr

Potential Saving and Benefits: Cloud HPC Service



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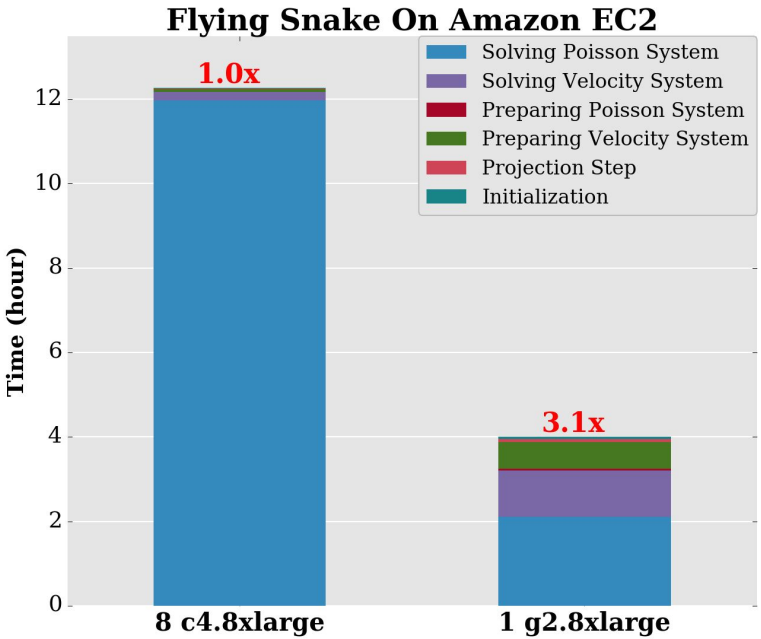
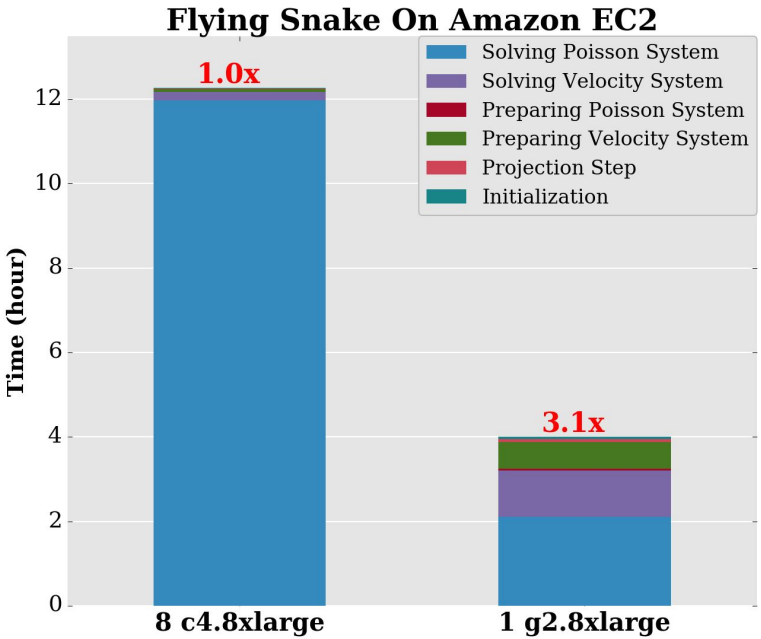


- **Using Spot Instances**
  - **CPU:**
    12.5 hr × $0.5† / hr × 8 nodes = **$50.0**

†This is the prices of the spot instances we used at that time.

Potential Saving and Benefits: Cloud HPC Service



- **Using Spot Instances**
  - **CPU:**
    12.5 hr × $1.675 / hr × 8 nodes = **$167.5**
  - **GPU:**
    4 hr × $2.6 / hr × 1 node = **$10.4**

Conclusion

- **AmgX and our wrapper**
  - https://developer.nvidia.com/amgx
  - https://github.com/barbagroup/AmgXWrapper
- **PetIBM with AmgX enabled:**
  - https://github.com/barbagroup/PetIBM/tree/AmgXSolvers
- **Time is money**
  - With AmgX and our wrapper, we save time on implementing multi-GPU capability into our existing PETSc-based applications
  - Multi-GPU capability shortens execution time and hardware resources needed
  - Less hardware resources reduce costs, works, and human resources

Thanks!

Acknowledgement:

Dr. Joe Eaton, NVIDIA

Contact us:

Website:
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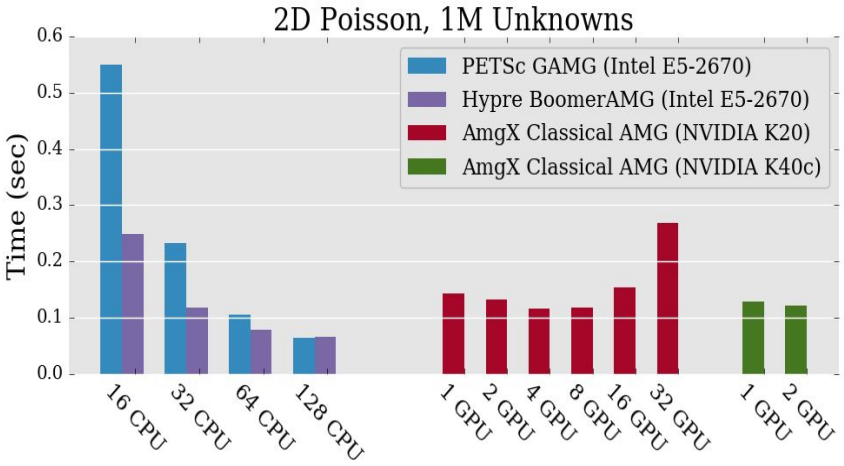
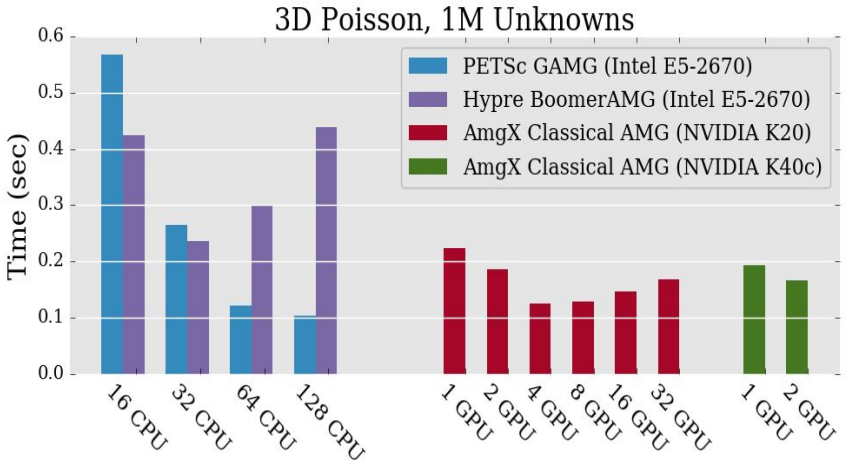
Q & A

Extra Slides

Example: Small-Size Problems





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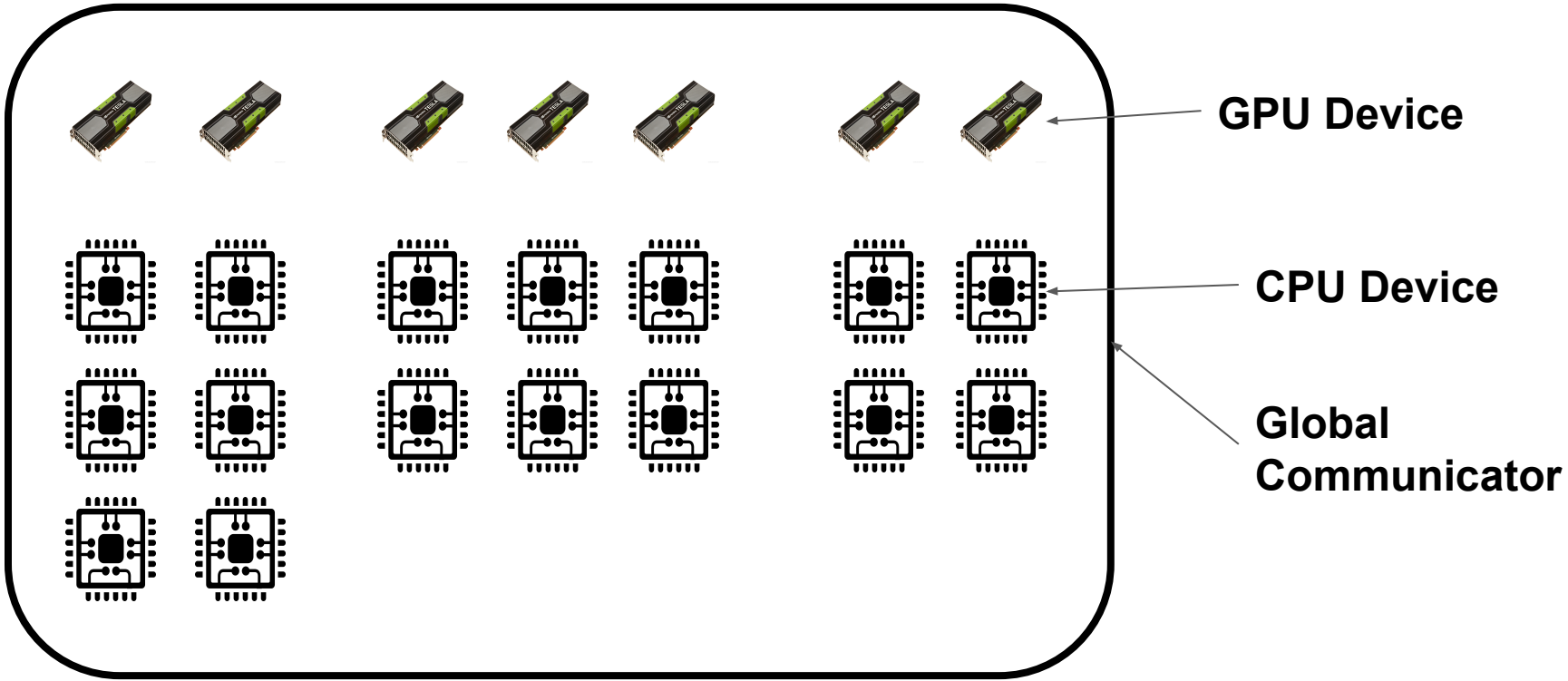

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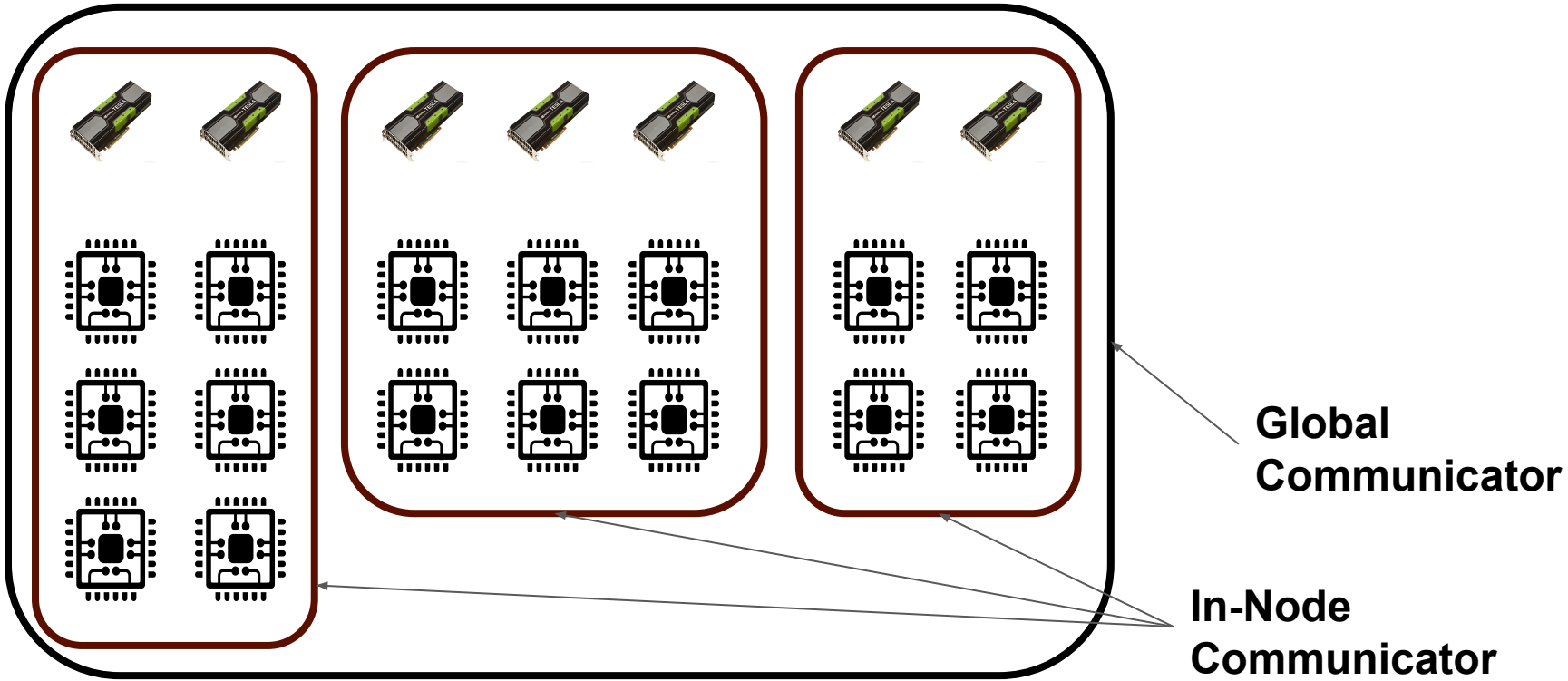

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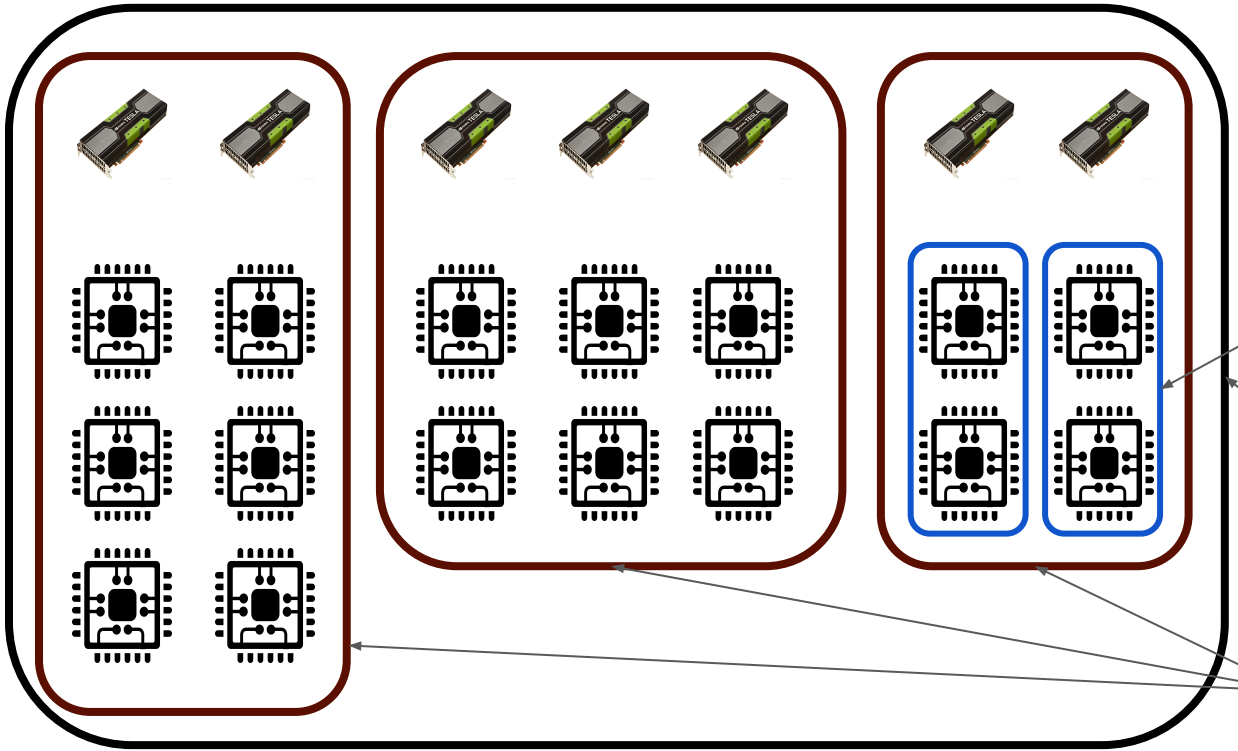

Matrix Consolidation Communicator

Global Communicator

In-Node Communicator

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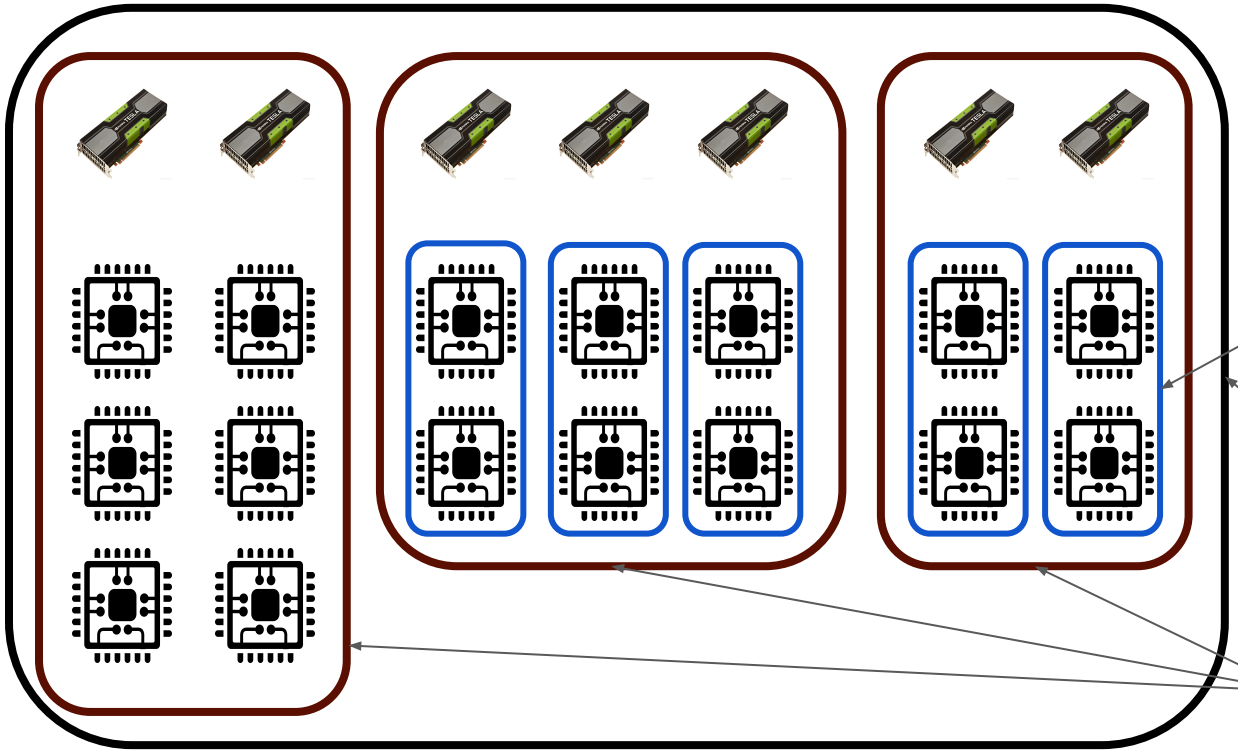

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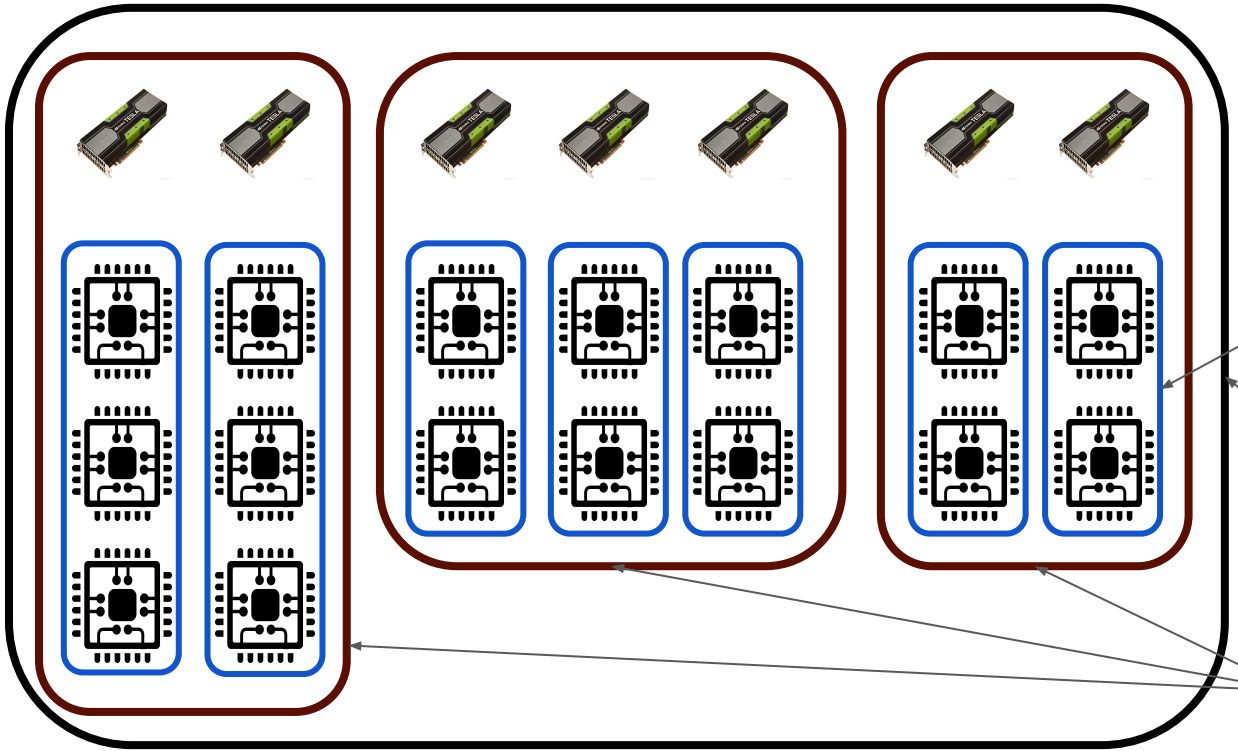

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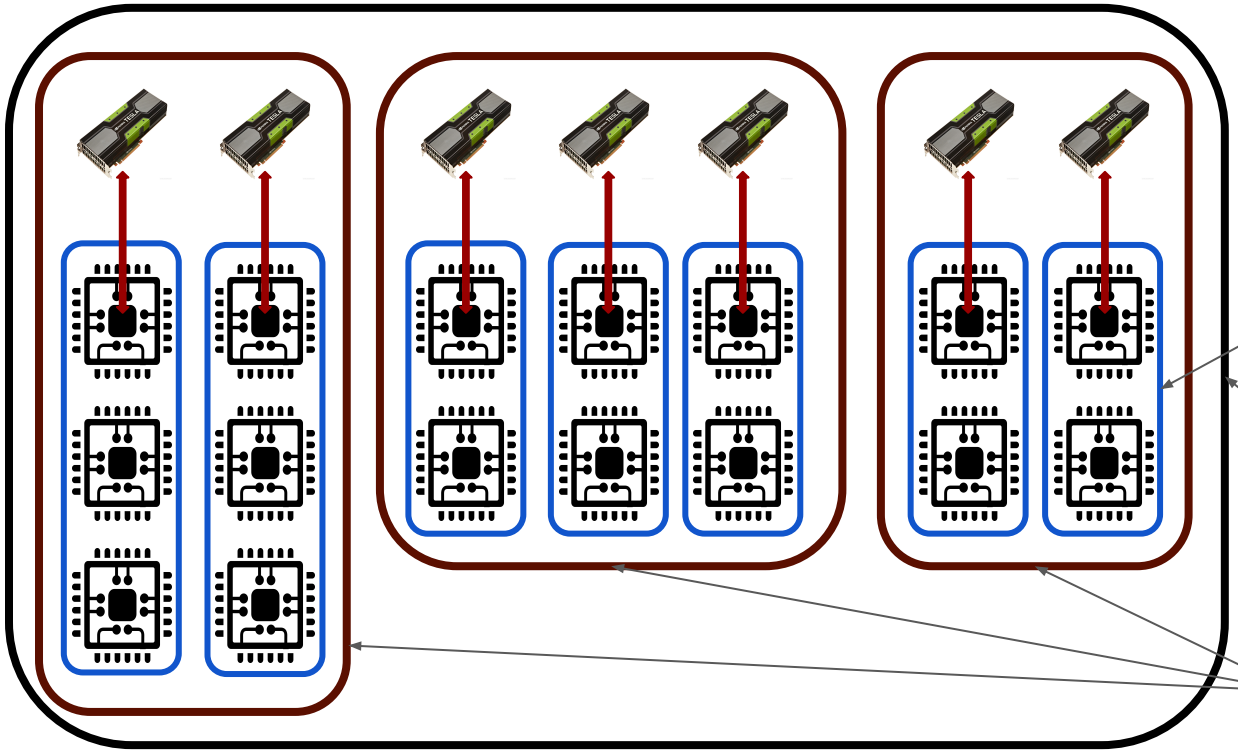

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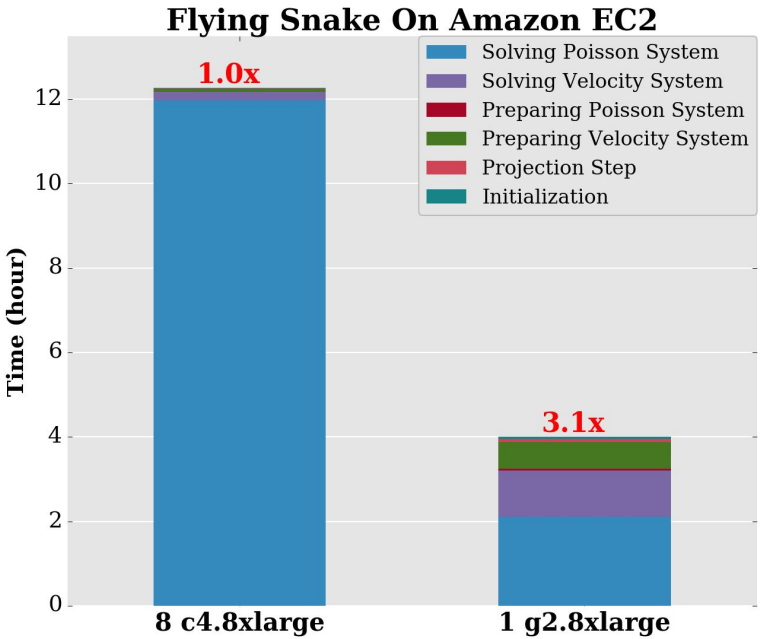
Potential Saving and Benefits: Cloud HPC Service



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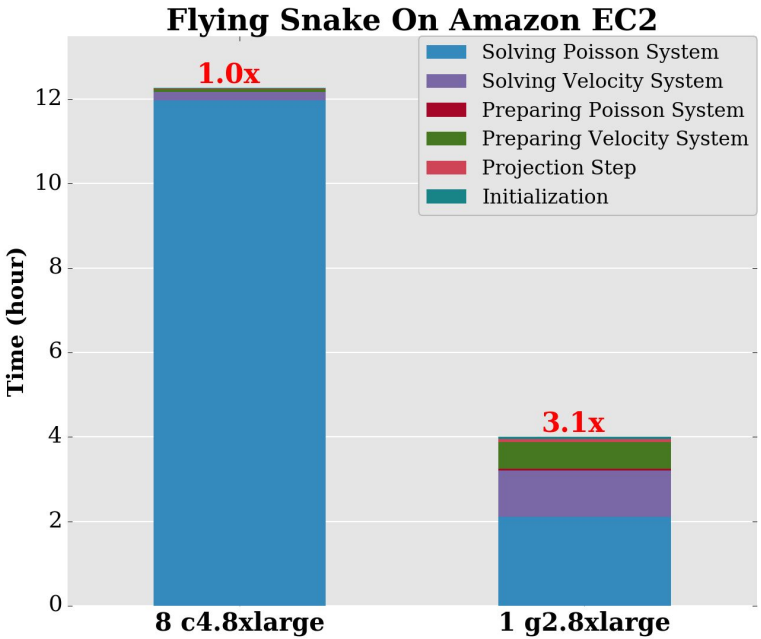

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