Productivity Challenges for Code Coupling in an HPC Environment

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Albuquerque, NM, USA

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Extreme-Scale Computing

- Trends: More FLOPS with comparatively less storage, I/O bandwidth
  - Consequence: A smaller fraction of data can be captured on disk

Oak Ridge National Laboratory

	System Peak	I/O BW
Jaguar (2008)	263 TFLOPS	44 GB/s
Jaguar PF (2009)	1.75 PFLOPS	240 GB/s
Titan (2012)	20 PFLOPS	240 GB/s
Factor Change	**76×**	**5.5×**

Bland, Kendall, Kothe, Rogers, and Shipman. "Jaguar: The World's Most Powerful Computer"
http://archive.hpcwire.com/hpcwire/2012-10-29/titan_sets_high-water_mark_for_gpu_supercomputing.html?featured=top

Argonne National Laboratory

	System Peak	I/O BW
Intrepid (2003)	560 TFLOPS	88 GB/s
Mira (2011)	10 PFLOPS	240 GB/s
Factor Change	**17.8×**	**2.7×**

https://www.alcf.anl.gov/intrepid
https://www.alcf.anl.gov/mira

Lawrence Livermore National Laboratory

	System Peak	I/O BW
ASC Purple (2005)	100 TFLOPS	106 GB/s
Sequioa (2012)	20 PFLOPS	1 TB/s
Factor Change	**200×**	**9.4×**

http://www.sandia.gov/supercomp/sc2002/flyers/SC02ASCIPurplev4.pdf
https://asc.llnl.gov/publications/Sequoia2012.pdf

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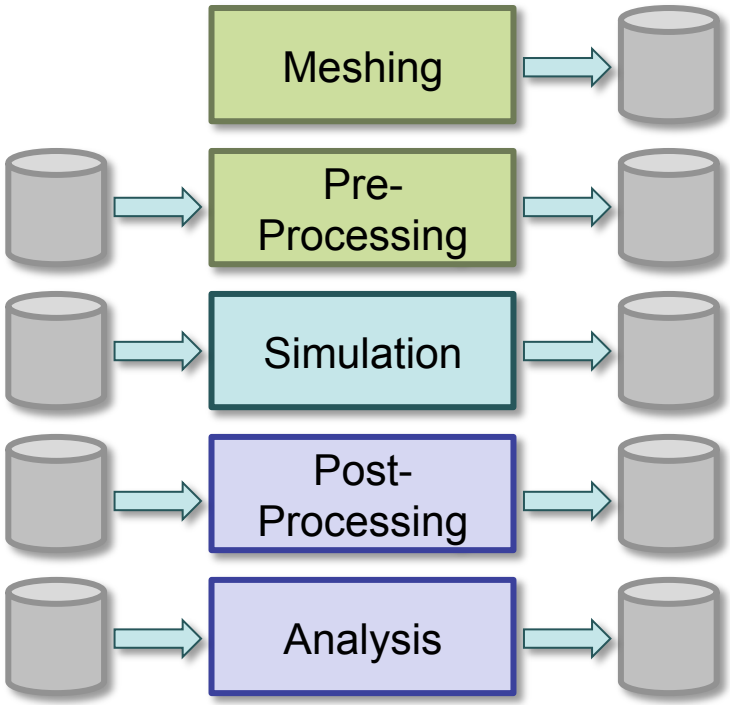
	System Peak	I/O BW
Red Storm (2003)	180 TFLOPS	100 GB/s
Cielo (2011)	1.4 PFLOPS	160 GB/s
Factor Change	**7.8×**	**1.6×**

https://cfwebprod.sandia.gov/cfdocs/CCIM/docs/033768p.pdf
http://www.lanl.gov/orgs/hpc/cielo/

Usage Models Conflict with Trends

App workflows historically use storage system for communication



One way to relieve I/O pressure is to integrate components

Two Approaches to Integration

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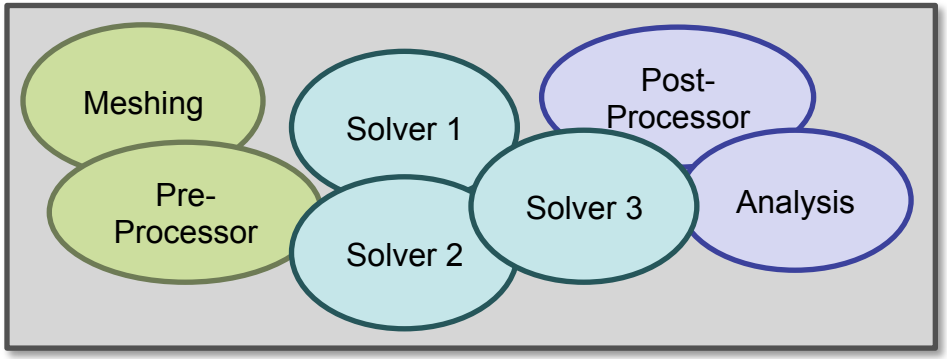
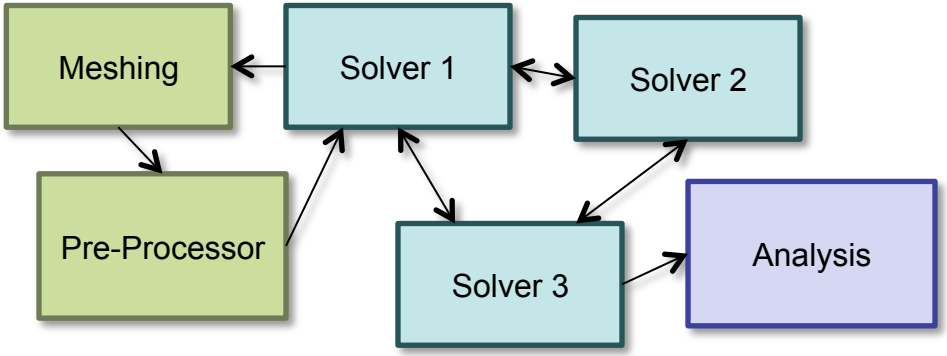
Tightly Coupled



- Pros
  - Standard communication (MPI)
  - Supported by HPC runtimes
- Productivity Challenges
  - Configuration/build (lib conflicts)
  - Data structure mismatches
  - Resilience (one fails, they all fail)

Loosely Coupled



- Pros
  - Configuration/build is easy
  - Resilience is easier to manage
- Productivity Challenges
  - Not well supported by runtimes
  - No dynamic scheduling, placement, load balancing, …
  - No standard comm interface

What People are Doing

- OS and Runtime changes to support integrated workflows
  - Hobbes and Argo – Both ASCR projects
  - Resource management, data sharing, application composition, prog models.
- Software frameworks for composing integrated workflows
  - Network Scalable Service Interface (Nessie) – SNL
  - Adaptable I/O System (ADIOS) – ORNL, GA Tech
- Nessie Network Transport Interface (NNTI)
  - Portable RDMA abstraction (Cray XT/XE, IBM BG, InfiniBand)
  - Used by Nessie and ADIOS
- Tightly Coupled Codes and In-situ Analysis and Visualization
  - CASL (simulation of light water reactors)
  - ParaView/Catalyst (SNL/Kitware)
  - GLEAN (ANL)
- TriBits
  - Build integrate and test system – Designed to ease the configuration burden

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