“I have had my results for a long time, but I do not yet know how I am to arrive at them.”
–Carl Friedrich Gauss, 1777-1855

Imaging Meets HPC Through Scalable Data Analysis

Reconstructed image of gold nanostructure with 30nm features
[courtesy Junjing Deng (NU) and Youssef Nashed (ANL)]
Definition of Data Analysis

- Any data transformation, or a network or transformations.
- Anything done to original data beyond its original generation.
- Can be visual, analytical, statistical, or data management.
Streamlines and pathlines
[Peterka et al. IPDPS’11]

FTLE
[Nouanesengsy et al. SC12]

Morse-Smale complex
[Gyulassy et al. IPDPS’12]

Stream surfaces
[Lu et al. SC14]

Information entropy
[Chaudhuri et al. LDAV’12]

Voronoi and Delaunay tessellation
[Peterka et al. SC14]

Ptychography
[Nashed et al. in submission]
Common Denominators

- Big science => big data, big machines
- Most analysis algorithms are not up to speed
  - Either serial, or
  - Overheads kill scalability
- Solutions
  - Process data closer to the source
  - Write scalable analysis algorithms
  - Parallelize in various forms
  - Build software stacks of useful and reusable layers
- Usability and workflow
  - Develop libraries rather than tools
  - Users write small main programs and call into libraries
### Abstractions Matter

#### Parallelizing by hand

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<tr>
<td>Stochastic</td>
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<tr>
<td>OS / Runtime</td>
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</table>

```c
void ParallelAlgorithm() {
    ...
    MPI_Send();
    ...
    MPI_Recv();
    ...
    MPI_Barrier();
    ...
    MPI_File_write();
}
```

#### With a data movement layer

<table>
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```c
void ParallelAlgorithm() {
    ...
    LocalAlgorithm();
    ...
    DIY_Merge_blocks();
    ...
    DIY_File_write()
}
```
Features of a Data Movement Layer

1. Separate analysis ops from data ops
2. Group data items into blocks
3. Assign blocks to processes
4. Group blocks into neighborhoods
5. Support multiple multiple instances of 2, 3, and 4
6. Handle time
7. Communicate between blocks in various ways
8. Read data and write results
9. Integrate with other libraries and tools
Many different analysis operations share a small set of communication patterns. These communication kernels together with supporting utilities for decomposition and I/O can be encapsulated, optimized, and reused.
3 Communication Patterns

Nearest neighbor

Round 0
k = 4

Round 1
k = 2

Results

Swap-based reduction

Merge-based reduction
Different Neighborhood Communication Patterns

DIY provides point to point and different varieties of collectives within a neighborhood via its enqueue_item mechanism. Items are enqueued and subsequently exchanged (2 steps).

How to enqueue items for neighbor exchange

- DIY offers several options
- Send to a particular neighbor or neighbors, send to all nearby neighbors, send to all neighbors
- Support for periodic boundary conditions involves tagging which neighbors are periodic and calling user-defined transform on objects being sent to them
DIY helps the user write data-parallel analysis algorithms by decomposing a problem into blocks and communicating items between blocks.

**Features**
- Parallel I/O to/from storage
- Domain decomposition
- Network communication
- Utilities

**Library**
- Written in C++ with C bindings
- Autoconf build system (configure, make, make install)
- Lightweight: `libdiy.a` 800KB
- Maintainable: ~15K lines of code, including examples

**DIY usage and library organization**
Writing a DIY Program

**Documentation**
- README for installation
- User’s manual with description, examples of custom datatypes, complete API reference

**Tutorial Examples**
- Block I/O: Reading data, writing analysis results
- Static: Merge-based, Swap-based reduction, Neighborhood exchange
- Time-varying: Neighborhood exchange
- Spare thread: Simulation and analysis overlap
- MOAB: Unstructured mesh data model
- VTK: Integrating DIY communication with VTK filters
- R: Integrating DIY communication with R stats algorithms
- Multimodel: multiple domains and communicating between them
Parallel Tessellation

We developed a prototype library for computing in situ Voronoi and Delaunay tessellations from particle data and applied it to cosmology, molecular dynamics, and plasma fusion.

**Key Ideas**

- Mesh tessellations convert sparse point data into continuous dense field data.
- Meshing output of simulations is data-intensive and requires supercomputing resources.
- No large-scale data-parallel tessellation tools exist.
- We developed such a library, tess.
- We achieved good parallel performance and scalability.
- Widespread GIS applicability in addition to the datasets we tested.
Strong and weak scaling for up to $2048^3$ synthetic particles and up to 128K processes (excluding I/O) shows up to 90% strong scaling and up to 98% weak scaling.
In simulations of microphase separated soft matter systems, populations of molecules self-organize to form two or more domains. Each domain contains only one type of bead. These domains can form complicated geometries such as the double gyroid.

We tessellated over 300 time steps of a system of 2,765 chains of an A-B-A triblock copolymer (176,960 total beads) found in an alternating gyroid morphology. Summing the Voronoi cells of the A and B species suggests that because the B part has to stretch or fold, the B domain dilates relative to the A domain.

The figure above shows the Voronoi tessellation of 1,000 A-B-C "telechelics" composed of two nanospheres (A and C) connected by a polymer tether beads (B) for a total of 8,000 beads in a double gyroid morphology. Only the Voronoi cells associated with the A species are shown. Such surfaces are usually constructed by using isosurface methods, which require averaging over many time steps; whereas by using the tessellation, such surfaces can be constructed for every time step.
Ptychographic Image Reconstruction

[Courtesy of Youssef Nashed, ANL]

An illustration of multi-GPU phase retrieval. The diffraction patterns are subdivided and distributed among available GPUs. Pairwise stitching is performed on the partial reconstructions attained by phase retrieval. The initial diffraction patterns are subdivided into DIY blocks merged together using DIY’s merge-based reduction communication pattern. Strong scaling efficiency on synthetic data is approximately 55% on 21,000 256x256 images.
Parallel Reconstruction Performance

[Courtesy of Youssef Nashed, ANL]

A gold Siemens star test pattern, with 30 nm smallest feature size, was raster scanned through a $26 \times 26$ grid using a step size of 40 nm and an exposure time of 0.6 s per scan point, using a 5.2 keV X-ray beam. The total scanning time was about 20 minutes.

![Image](a)  
(b)  
(c)  
(d)  

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**Strong Scaling on Real Data**

- **Wall time**
- **Perfect Scaling**

**Time (s)**

- 1000
- 100
- 10
- 1

**Number of GPUs**

- 1
- 2
- 4
- 8
- 16

---

**Performance Breakdown on Real Data**

- VO
- SPICE
- Merge

**Time (s)**

- 1000
- 100
- 10
- 1
- 0.1
- 0.01
- 0.001

**Number of GPUs**

- 1
- 2
- 4
- 8
- 16
Looking Ahead

A collaboration between ANL and LBL (Tom Peterka and Dmitriy Morozov) resulted both in new applications of DIY and a new prototype implementation of DIY2 featuring multithreaded in/out of core block management. Includes shared repositories (diy, diy2, tess, tess2) and publications [SC14].

Ongoing discussions between other ANL and LBL staff. (ANL: Peterka, Nashed, Jacobsen, Vine, McNulty; LBL: Ushizima, Krishnan, Shapiro, Marchesini, Maia, Sethian) regarding ptychographic reconstruction approaches.

[Courtesy of Dmitriy Morozov, LBL]

LBL (Dmitriy Morozov and Patrick O’Neil) developed tools for segmentation and connectivity analysis of granular and porous media using diy2.

Left: 3D image of a granular material (flexible sandstone) acquired at ALS by Michael Manga and Dula Parkinson. (Data: 2560 × 2560 × 1276). Right: Watershed segmentation of the material identifies individual grains (run on Edison @ NERSC) [courtesy Morozov, O’Neil (LBL)].
Further Reading

**DIY**
- Peterka, T., Ross, R.: Versatile Communication Algorithms for Data Analysis. 2012 EuroMPI Special Session on Improving MPI User and Developer Interaction IMUDI'12, Vienna, AT.

**DIY applications**
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People
Dmitriy Morozov (LBL)

https://bitbucket.org/diatomic/diy

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