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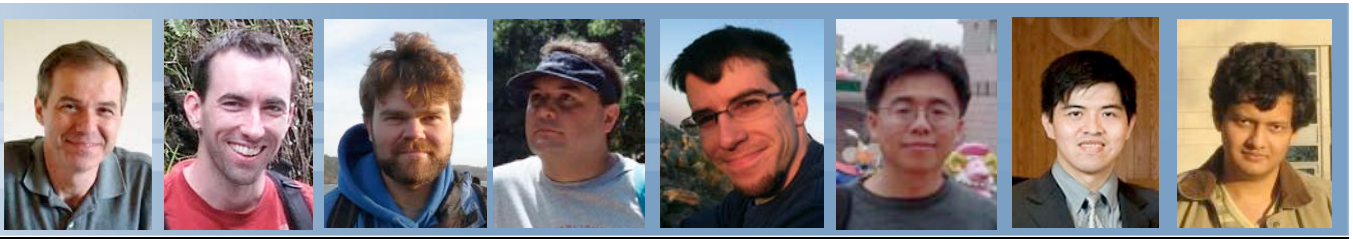

Scalable Parallel Building Blocks for Custom Data Analysis

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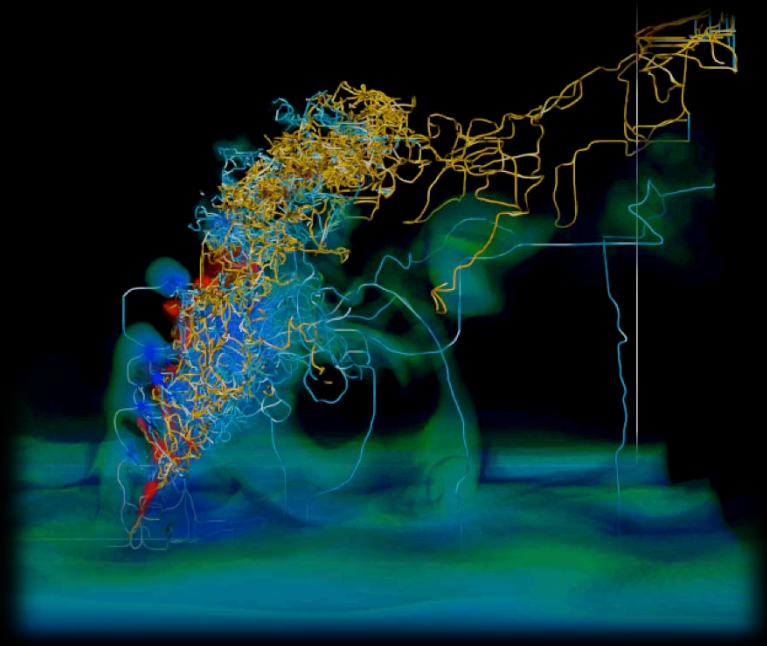
Wes Kendall (UTK)
Han-Wei Shen, Teng-Yok Lee, Abon Chaudhuri (OSU)

Morse-Smale Complex of combustion in the presence of a cross flow



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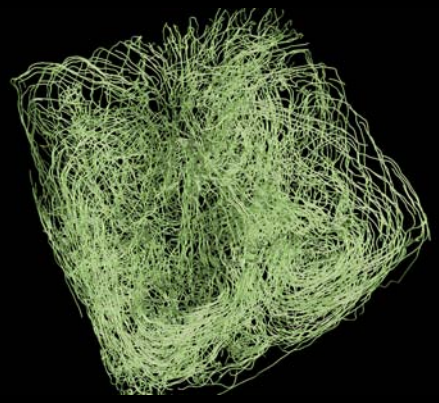
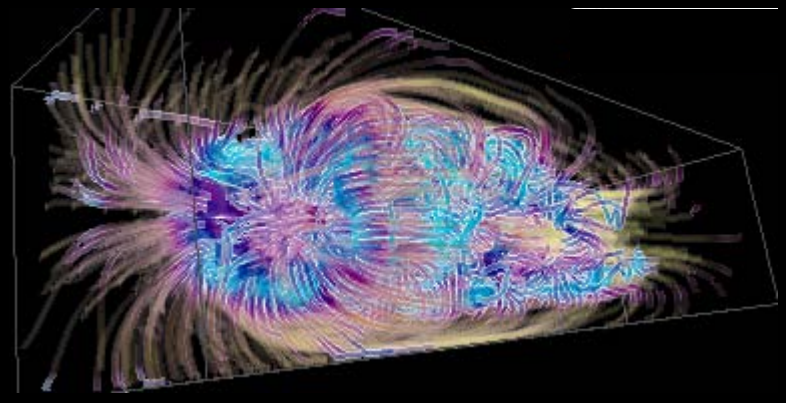
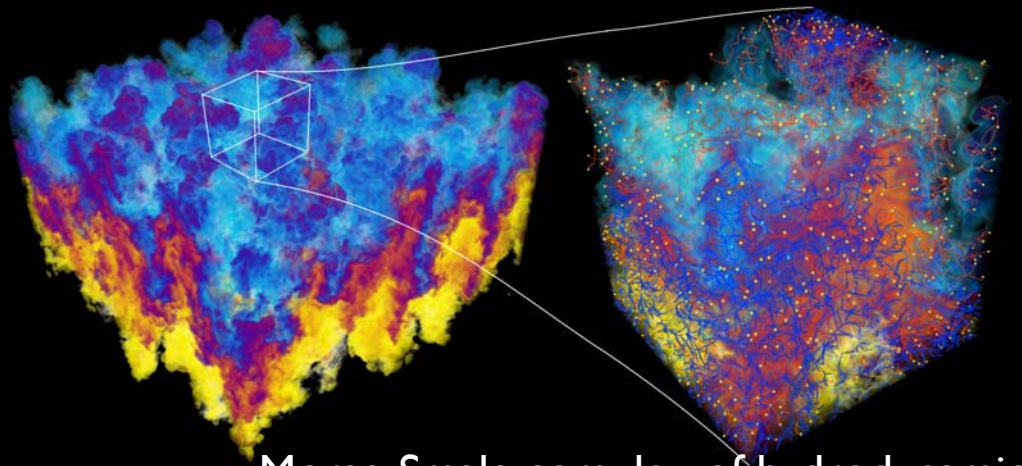
Survey of Science and Analysis Applications

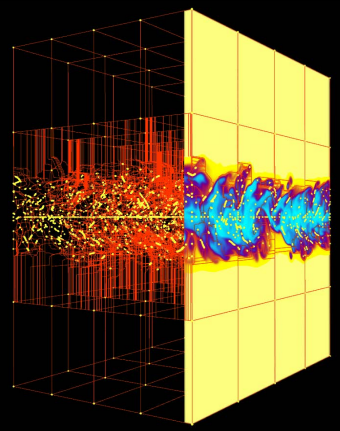


Particle tracing of thermal hydraulics flow



Information entropy analysis of astrophysics





Morse-Smale complex of hydrodynamics and combustion

-No two analyses are alike

-Analysis at scale is data-movement bound

-Data movement operations are common among different analyses

Executive Summary

DIY helps the user parallelize their analysis algorithm with data movement tools.

High-level motivations and assumptions

-Large-scale analysis (visual and numerical) in parallel on distributed-memory HPC machines

-Scientists, visualization researchers, tool builders

-In situ, coprocessing, postprocessing

-Parallelizing from scratch is arduous

-Scalable data movement is key

-The user is the expert and may already have serial code for the analysis.

A common set of operations can be identified and encoded in a library

-Decompose the domain

-Assign subdomains to processors

-Access data and store results

-Combine local and global operations

-Balance load, minimize communication

-Overlap communication with computation

-Scale efficiently

Benefits

-Researchers can focus on their own work, not on building parallel infrastructure

-Analysis applications can be custom

-Reuse core components and algorithms for performance and programmer productivity

DIY Structure

Features

Parallel I/O to/from storage

-MPI-IO, BIL

Domain decomposition

-Decompose domain

-Describe existing decomposition

Network communication

-Global reduction (2 flavors)

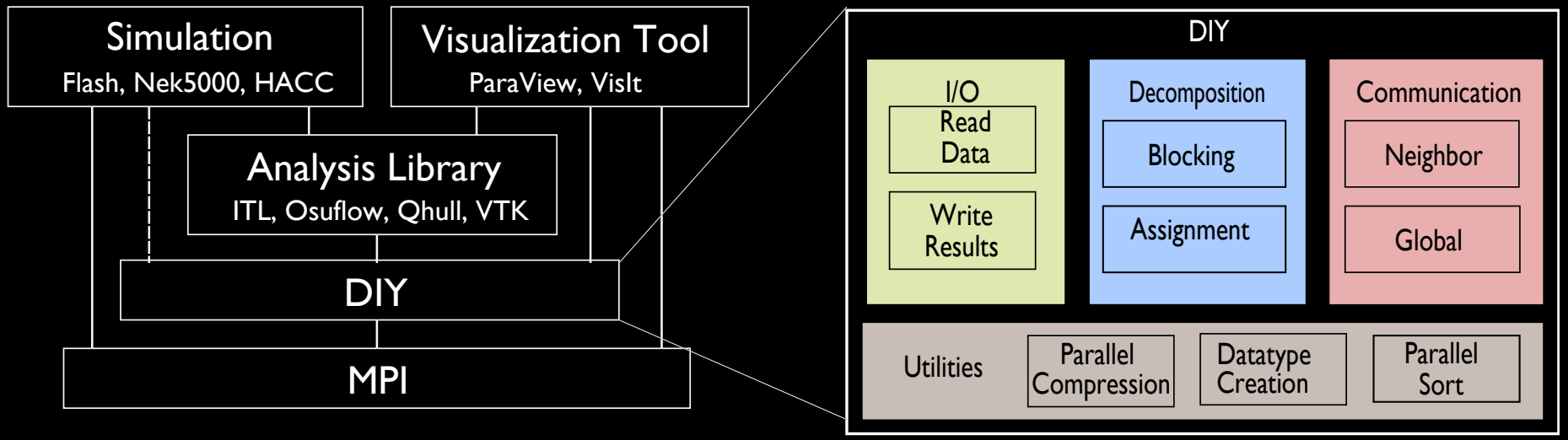
-Local nearest neighbor

Library structure

Written in C++

C bindings

Future Fortran bindings



DIY usage and library organization

Data Model

Features

-All input data and output analysis data is represented as MPI data types

-MPI data types can represent any C/C++/Fortran language structure

-User does not serialize / deserialize types prior to use

-Zero copy at application level saves time and space

-Custom MPI data types are an advanced topic

-DIY assists in MPI data type creation

C data structure

```
struct Particle {
 float[4] pt;
 int steps;
};
```

DIY MPI data type

```
MPI_Datatype type;
struct map_block_t map[] = {
 {MPI_FLOAT,  OFST,  4,  offsetof(struct Particle, pt),     1},
 {MPI_INT,    OFST,  1,  offsetof(struct Particle, steps),  1},
};
DIY_Create_datatype(0, 2, map, &type);
```

I/O: Parallel Reading Data and Writing Analysis Results

Data input

-Application-level two-phase I/O

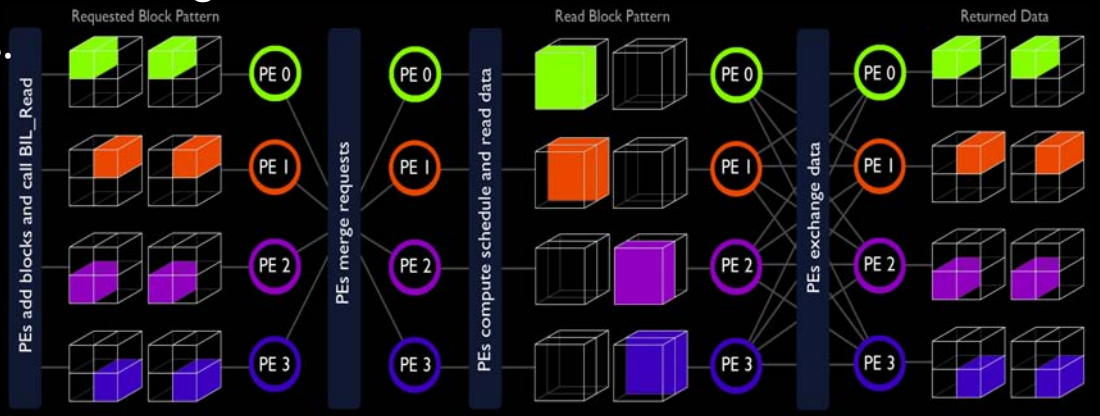
-Reads raw, netCDF, HDF5 (future)

-Read requests sorted and aggregated into large contiguous accesses

-Data redistributed to processes after reading

-Single and multi block/file domains.

Input algorithm



Analysis output

-Binary

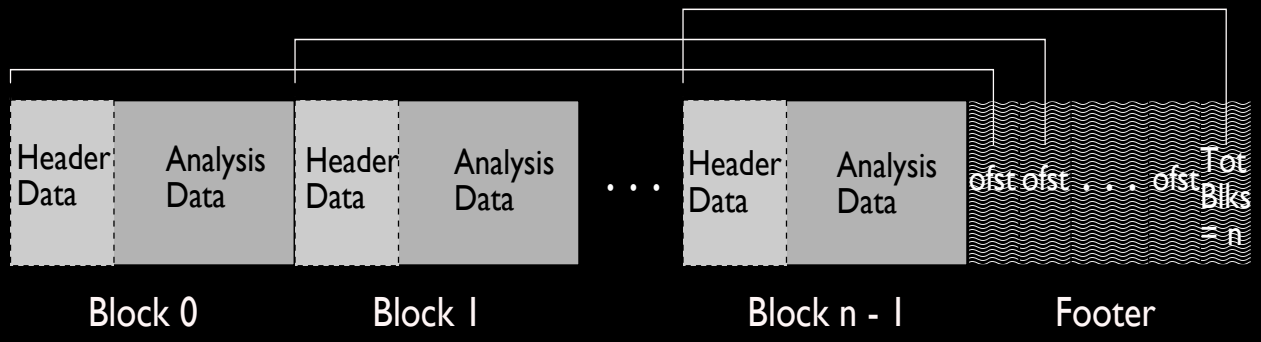
-General header/data blocks

-Footer with indices

-Application assigns semantic value to DIY blocks

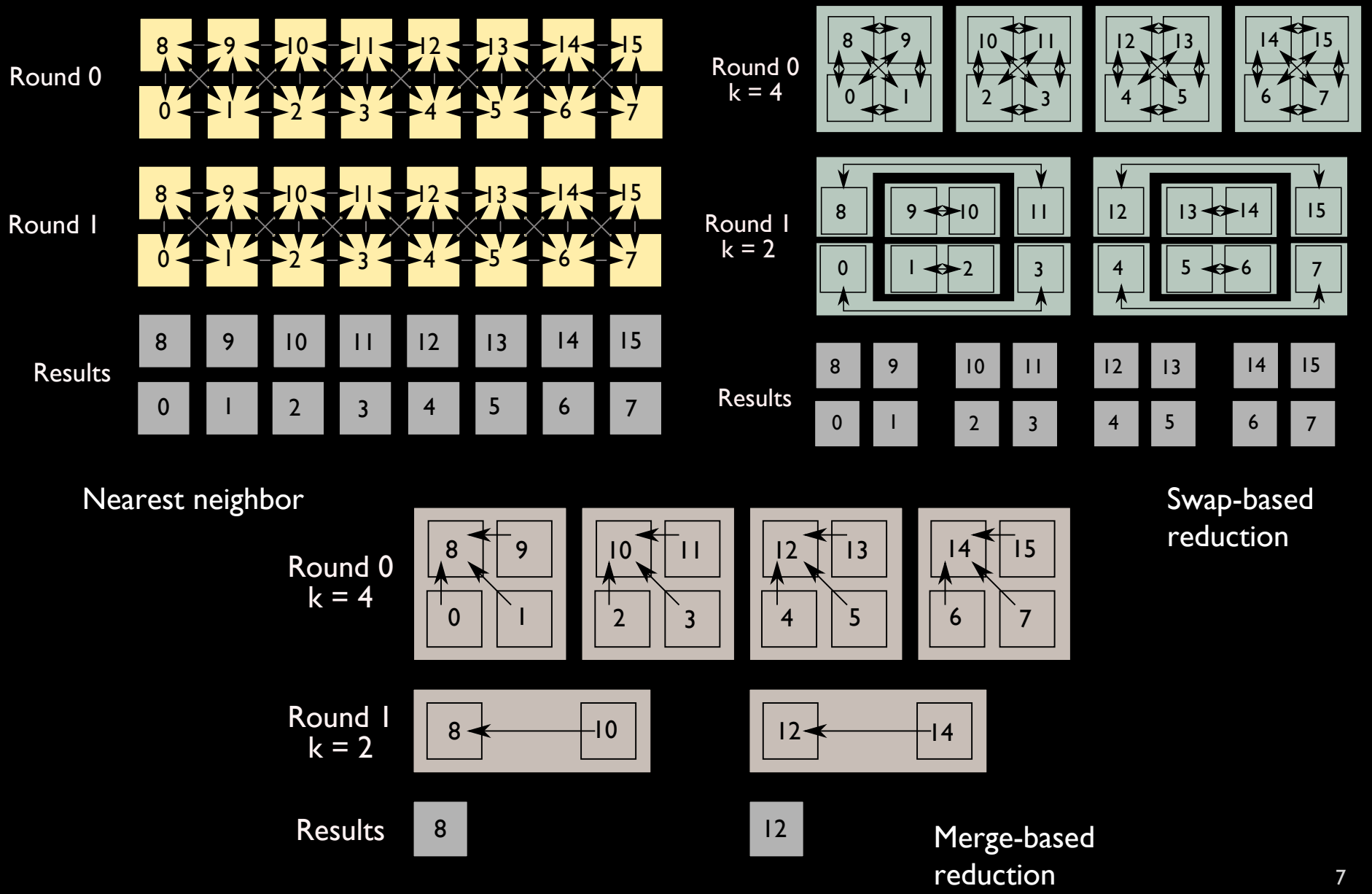
-Compression

Output file format



Kendall et al., Towards a General I/O Layer for Parallel Visualization Applications, CG&A '11

3 Communication Patterns



Example API Use

```
// initialize
int dim = 3; // number of dimensions in the problem
int tot_blocks = 8; // total number of blocks
int data_size[3] = {10, 10, 10}; // data size
MPI_Init(&argc, &argv); // init MPI before DIY
DIY_Init(dim, ROUND_ROBIN_ORDER, tot_blocks, &nblocks, data_size,
    MPI_COMM_WORLD);

// decompose domain
int share_face = 0; // whether adjoining blocks share the same face
int ghost = 0; // besides sharing a face, whether additional layers of ghost cells are needed
int ghost_dir = 0; // ghost cells apply to all or particular sides of a block
int given[3] = {0, 0, 0}; // constraints on blocking (none)
DIY_Decompose(share_face, ghost, ghost_dir, given);

// read data
 for (int i = 0; i < nblocks; i++) {
    DIY_Block_starts_sizes(i, min, size);
    DIY_Read_add_block_raw(min, size, infile, MPI_INT, (void**)&(data[i]));
}
DIY_Read_blocks_all();
```

Example API Continued

```
// your own local analysis

// merge results, in this example
// could be any combination / repetition of the three communication patterns
int rounds = 2; // two rounds of merging
int kvalues[2] = {4, 2}; // k-way merging, eg 4-way followed by 2-way merge
int nb_merged; // number of output merged blocks
DIY_Merge_blocks(in_blocks, hdrs, num_in_blocks, out_blocks, num_rounds, k_values,
&MergeFunc, &CreateItemFunc, &DeleteItemFunc, &CreateTypeFunc, &num_out_blocks);


  // write results
  DIY_Write_open_all(outfile);
  DIY_Write_blocks_all(out_blocks, num_out_blocks, datatype);
  DIY_Write_close_all();

  // terminate
  DIY_Finalize(); // finalize DIY before MPI
  MPI_Finalize();
```

Parallel Time-Varying Flow Analysis

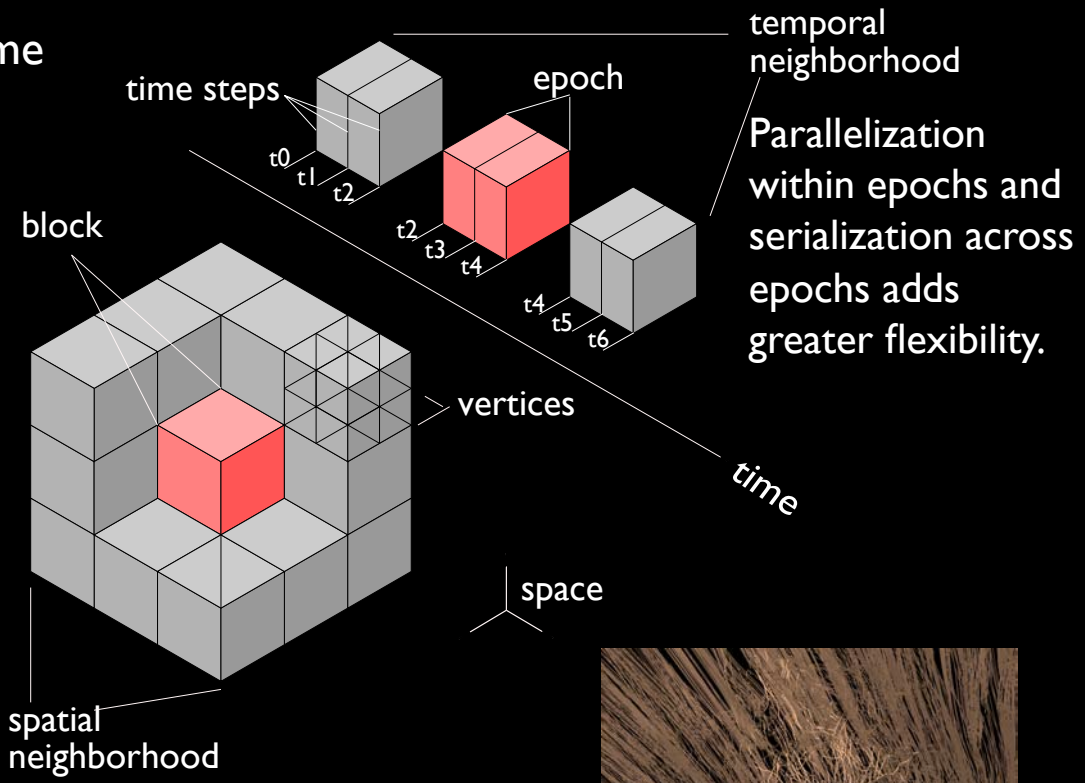
Collaboration with the Ohio State University and University of Tennessee Knoxville

Approach

-In core / out of core processing of time steps

-Simple load balancing (multiblock assignment, early particle termination)

-Adjustable synchronization communication



Parallelization within epochs and serialization across epochs adds greater flexibility.

Algorithm

```
for (epochs) {
  read my process' data blocks
  for (rounds) {
    for (my blocks) {
      advect particles
    }
    exchange particles
  }
}
```

Pathline tracing of 32 time-steps of combustion in the presence of a cross-flow

Peterka et al., A Study of Parallel Particle Tracing for Steady-State and Time-Varying Flow Fields, IPDPS '11

Parallel Information-Theoretic Analysis

Collaboration with the Ohio State University and New York University Polytechnic Institute

Objective

-Decide what data are the most essential for analysis

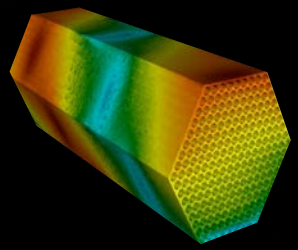
-Minimize the information losses and maximize the quality of analysis

-Steer the analysis of data based on information saliency

Information-theoretic approach

-Quantify Information content based on Shannon's entropy

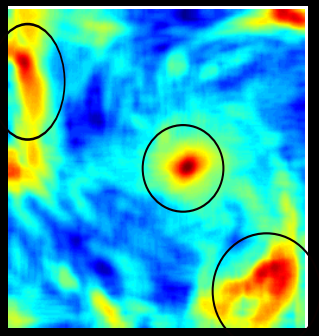
-Use this model to design new analysis data structures and algorithms



Nek5000
CFD model

Information-
theoretic
algorithms

Areas of high information entropy--turbulent regions in original data--are the interesting regions in simulating coolant flow in a nuclear reactor.



Section of information entropy field

Shannon's Entropy

The average amount of information expressed by the random variable is

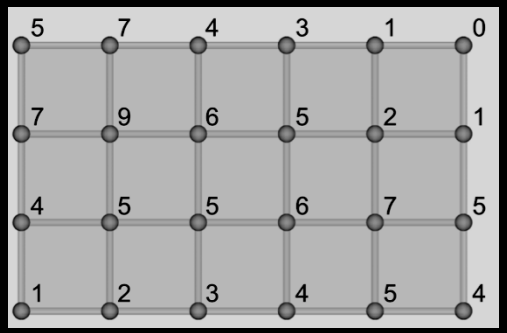
$$H(x) = -\sum_{i=1}^{n} p_i \log p_i$$

Parallel Topological Analysis

Collaboration with SCI Institute, University of Utah

-Transform discrete scalar field into Morse-Smale complex
-Nodes are minima, maxima, saddle points of scalar values
-Arcs represent constant-sign gradient flow
-Used to quickly see topological structure

1



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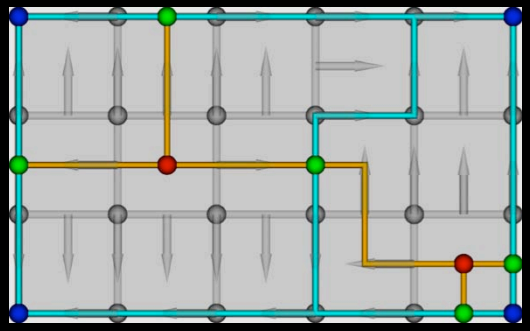

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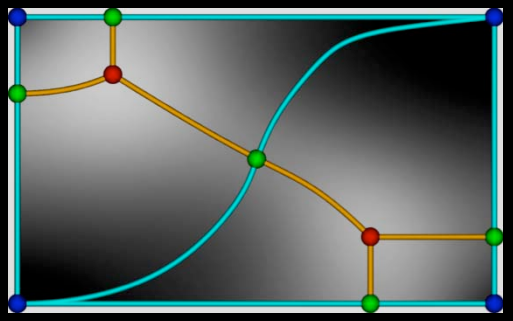

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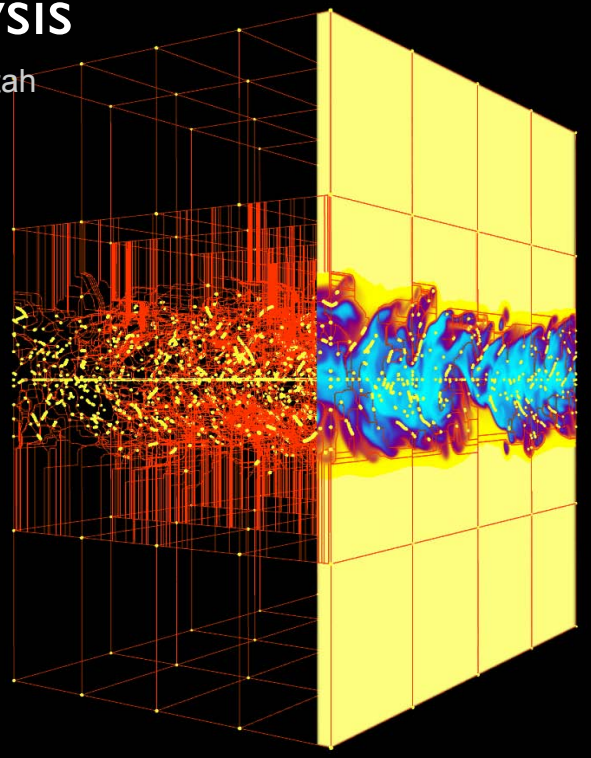
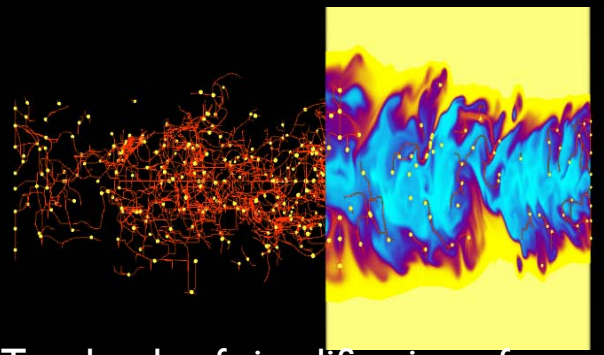
Example of computing discrete gradient and Morse-Smale Complex

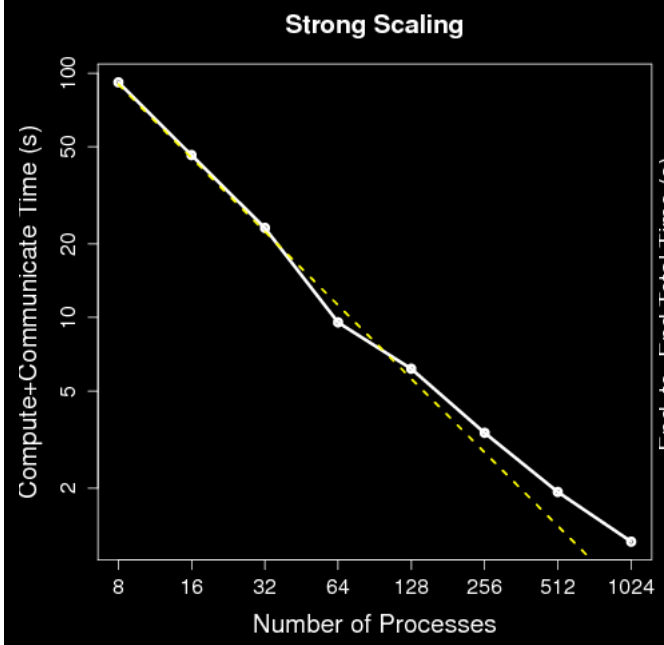


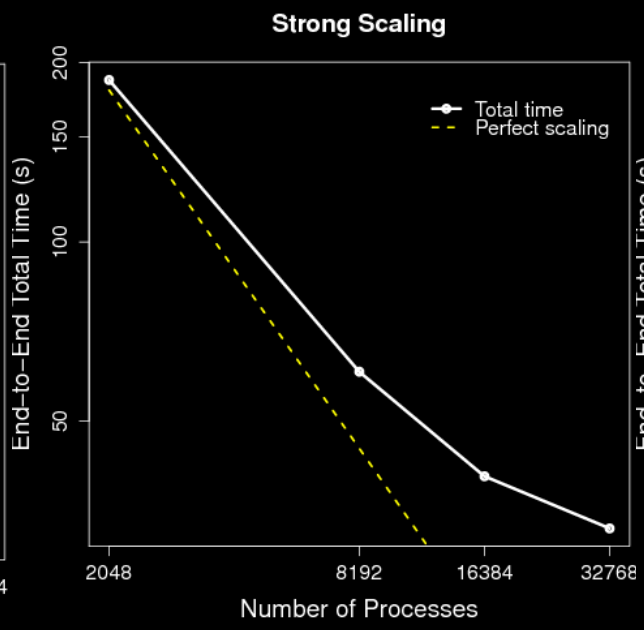


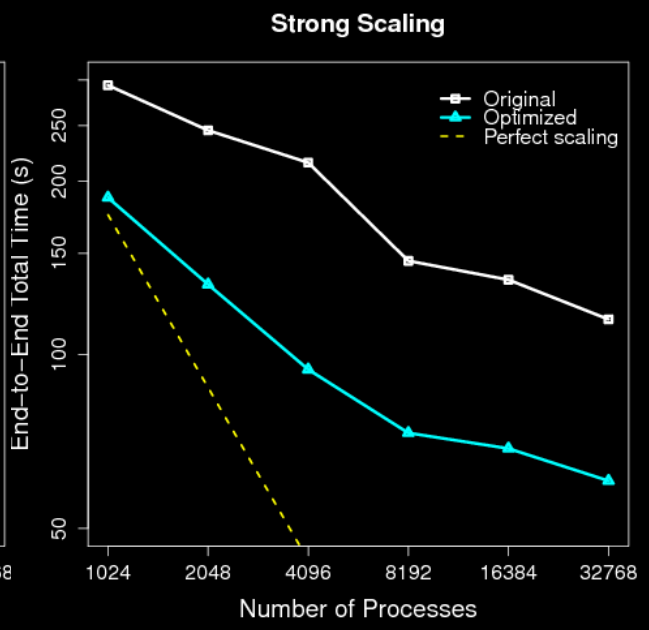
Two levels of simplification of the Morse-Smale complex for jet mixture fraction.

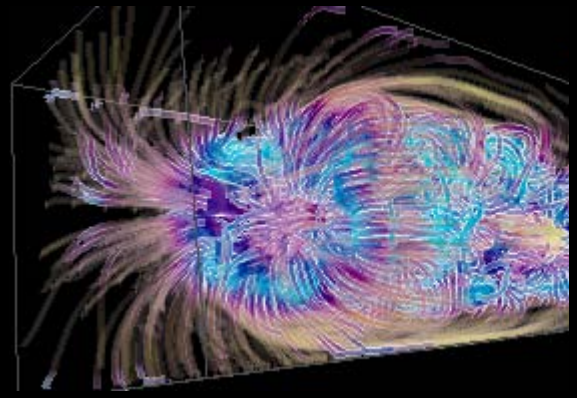
Gyulassy et al., The Parallel Computation of Morse-Smale Complexes, Submitted to IPDPS '12

Performance and Scalability

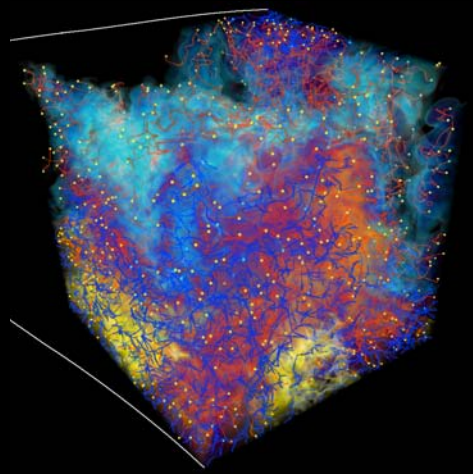




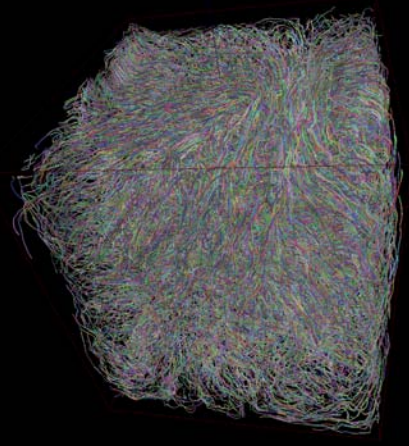




Information entropy



Topological analysis



Particle tracing

Summary

Main ideas

-Scalable analysis is about moving, transforming, reducing, analyzing, storing data

-Scientists, researchers take ownership of their own analysis

Successes

-Supports numerous, diverse analysis techniques

-Enables serial algorithms to be parallelized

-Flexible combination of data movements

-Both postprocessing and in situ

-Efficient and scalable

Limitations

-Requires effort on the part of the user

-Needs a program and (expert?) programmer

Ongoing

Finish installing existing code for swap-based reduction

AMR, unstructured, particle decomposition

Hybrid parallelism?

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"The purpose of computing is insight, not numbers."

–Richard Hamming, 1962

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ANL LDRD

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