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# Rendezvous algorithms for large-scale particle sim

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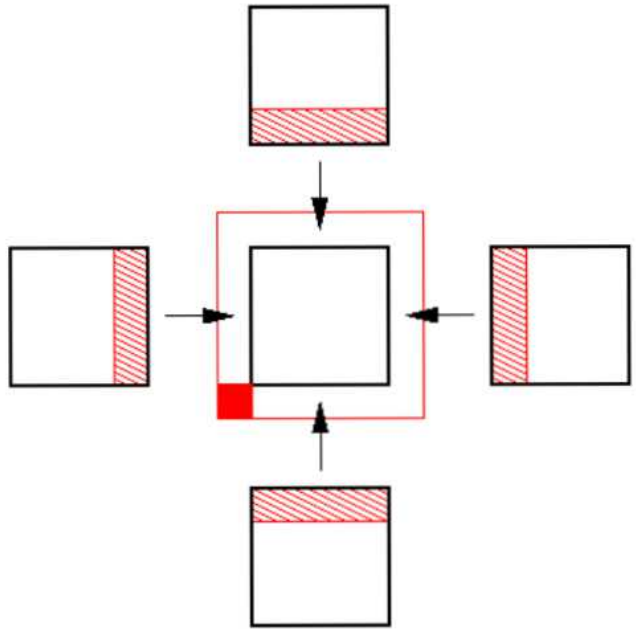
# Communication patterns

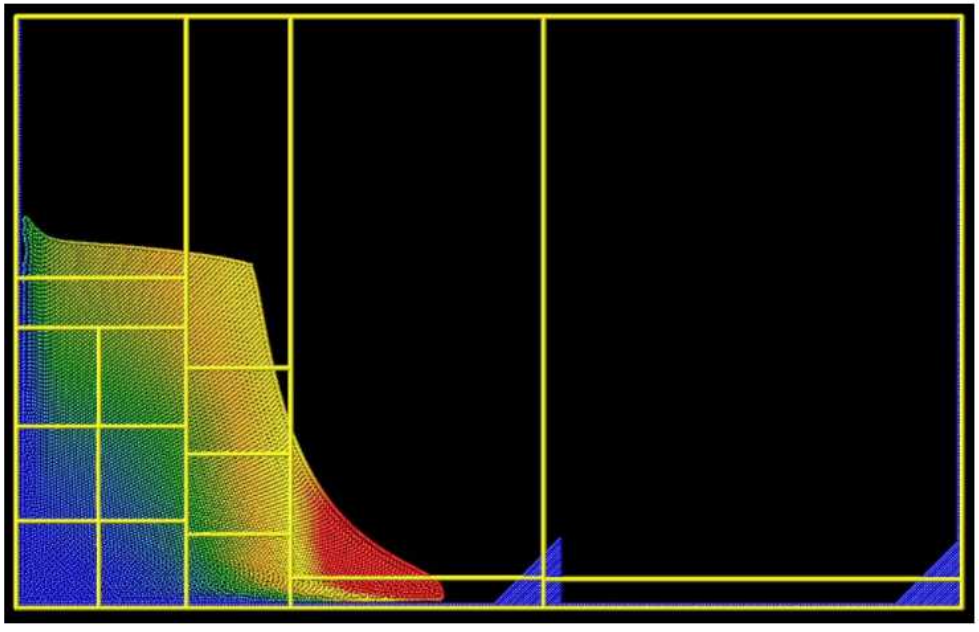
(1) Regular, often structured

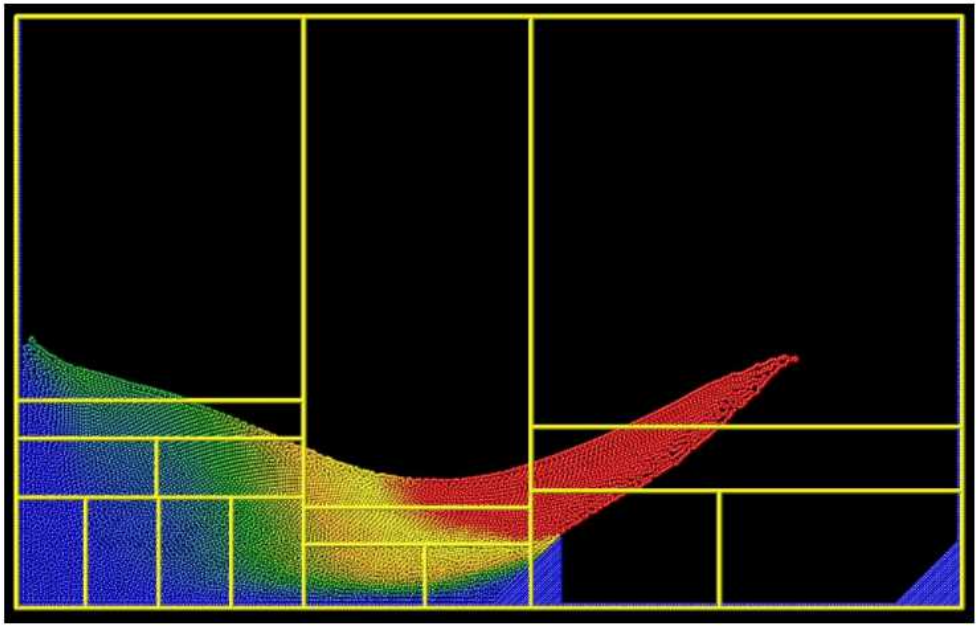
- Procs **know** who to **send** to,
  and who to **receive** from
- Domain decomp,
  halo of ghost cells or particles
- Exchange with
  4 or 8 procs in 2d, 6 or 26 in 3d
- MPI:
  Send(), Recv(), Irecv(), Sendrecv()



# Communication patterns

(2) Irregular, often unstructured





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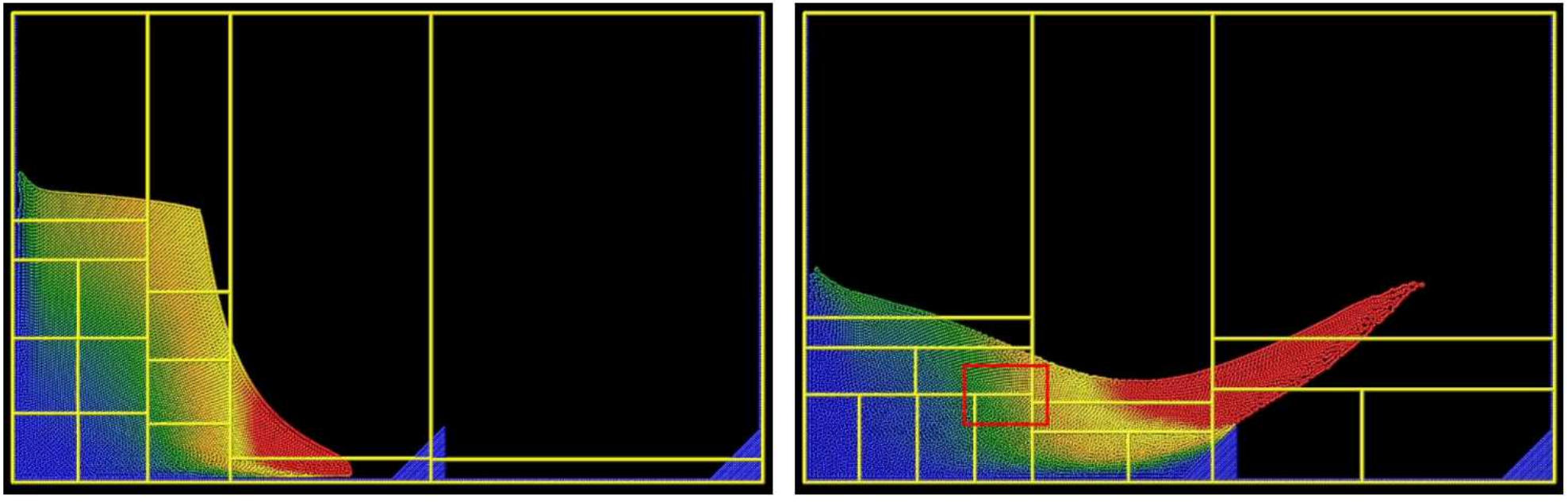

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- Procs **know** who to **send** to, but **not** who to **receive** from
- Load rebalance: send my data to new owning procs
- Comm with small, but arbitrary # of other procs
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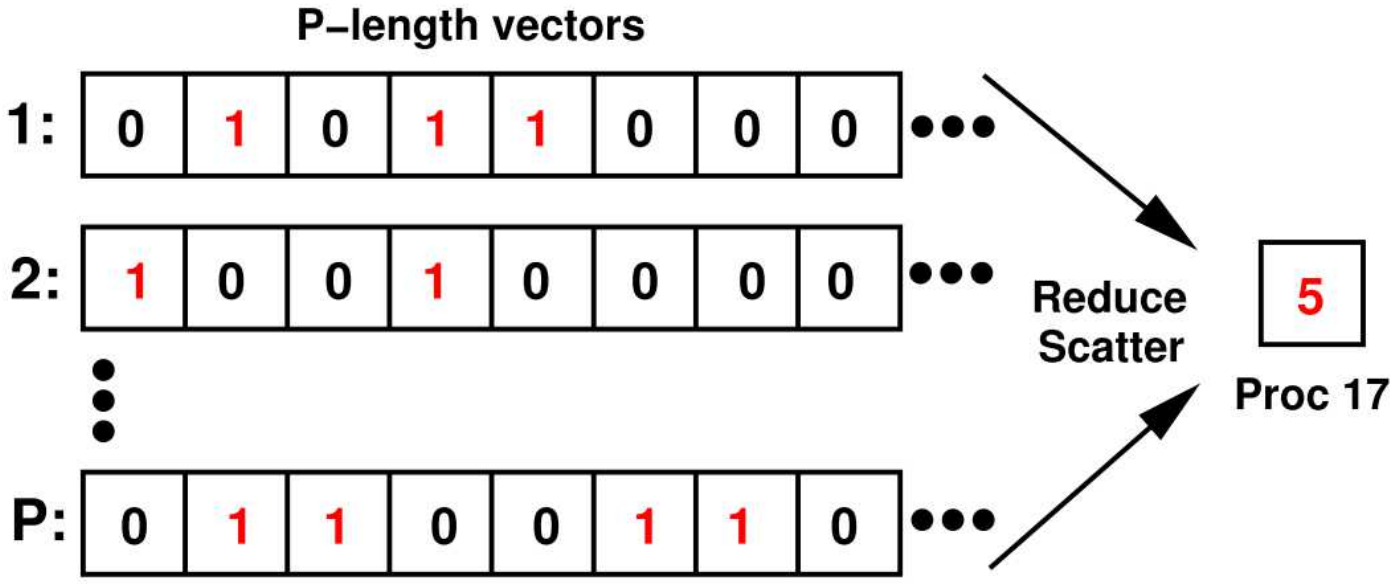

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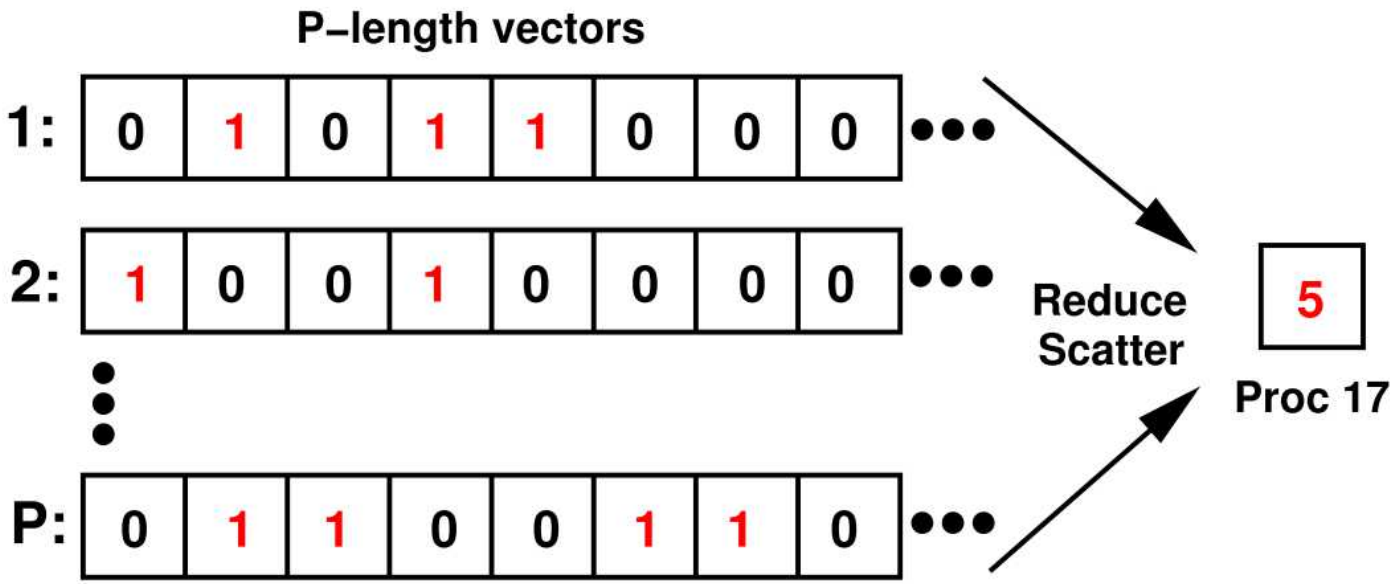


- Trilinos and Zoltan packages use this pattern

# Another communication pattern

(3) Rendezvous

- Procs **don't know** who to **send** to, **nor** who to **receive** from
- **Key idea**: create an **intermediate decomposition**
- Procs know who to send to (in Rvous decomp)
- Procs know who to receive from (sent from Rvous decomp)
- Often random comm with a few or nearly all procs
- Randomization **load balances** the comm and comp
- MPI: Reduce_scatter() or All2all()

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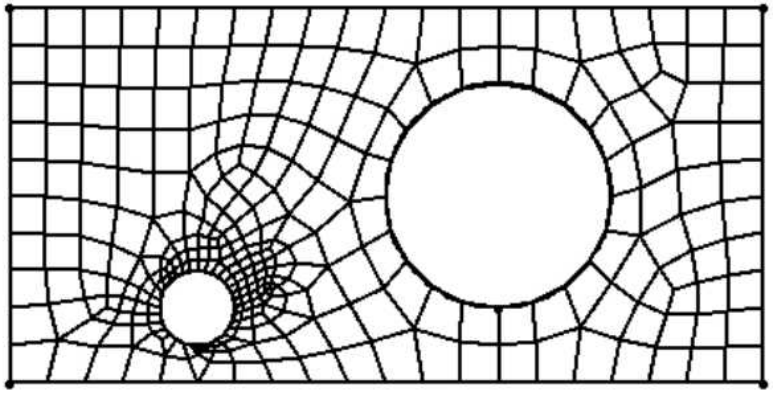
Why call it a **rendezvous algorithm**?

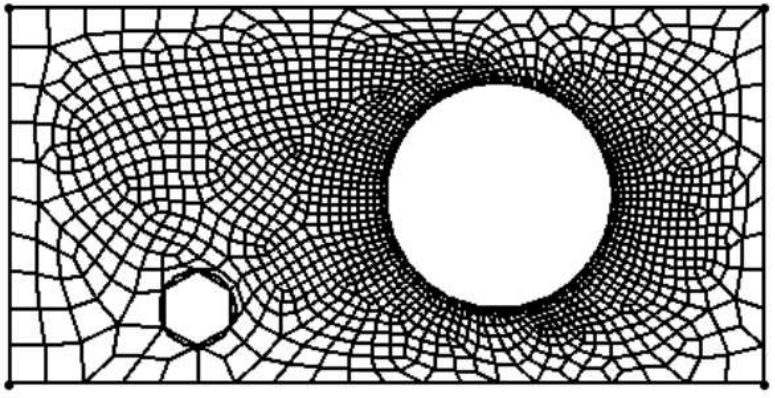
Because datums from different procs **rendezvous** at a single proc, so that proc can perform a computation that needs all the datums

# Rendezvous algorithm for grid transfer operation

*Plimpton, Hendrickson, Stewart, "A Parallel Rendezvous Algorithm for Interpolation Between Multiple Grids", J Parallel and Distributed Computing, 64, 266-276 (2004).*



**thermal**



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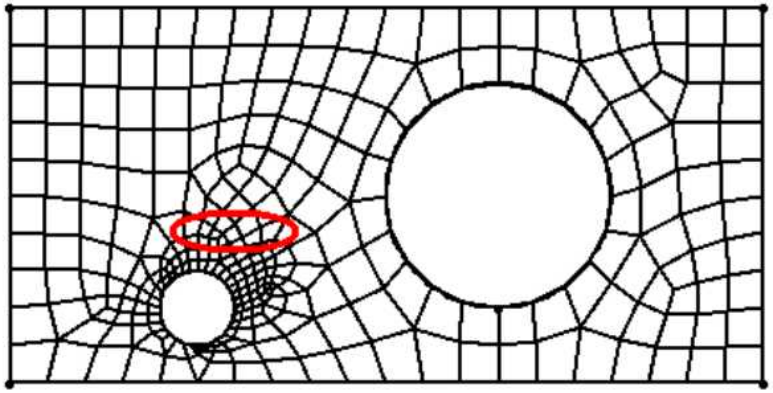

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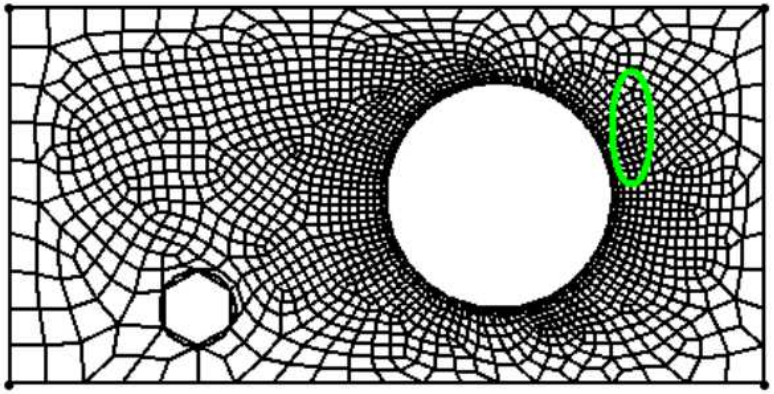
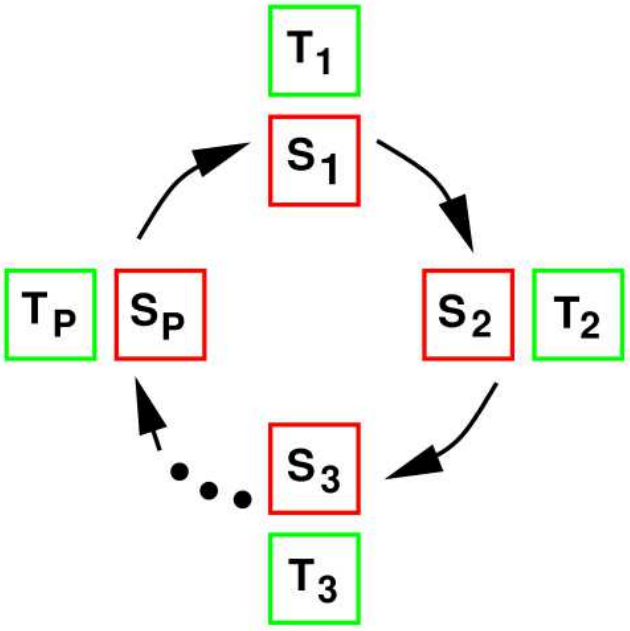


**stress**

- Two grids overlay same physical domain
- Refined & decomposed independently for physics & efficiency
- Each proc owns a random sub-domain in **both** decomps
- Interpolate between 2 grids, back-and-forth each timestep
- T⇒S requires data from all T procs which overlap a S proc
- But procs **know nothing** about either global decomposition

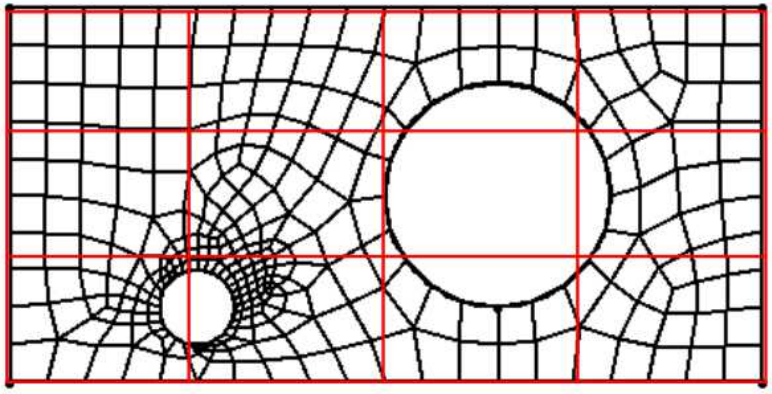
# Brute force solution

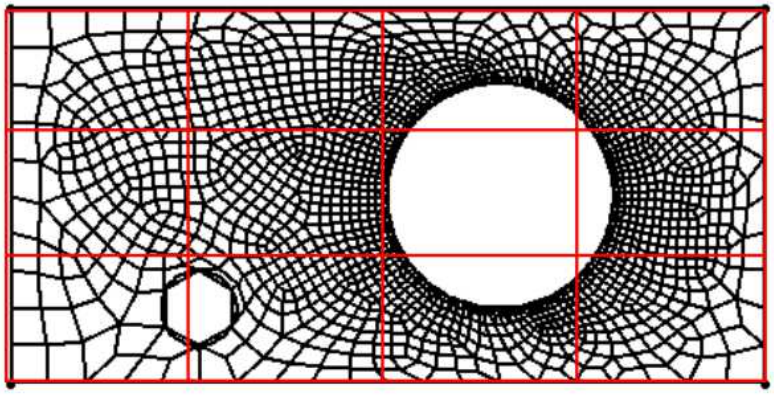
**Ring** communication:




- **Circulate** my S decomp grid cells **around ring to all procs**
- Each receive: keep S cells that overlap my T cells
- After P steps, each T proc can now perform interpolation
- Comp scaling: examine all N grid cells $\Rightarrow$ O(N)
- Comm scaling: P messages of size N/P $\Rightarrow$ O(N)
- **If occasional**, simple and actually OK for modest N and P
- But not for **huge N or P** or every step

# Rendezvous solution





- Create a geometrically-based **rendezvous decomp** R
- Regular grid of procs, or RCB (for load balancing)
- **Important**: all procs are part of all 3 decomps: S,T,R
- T procs: send info for each grid cell to owning R proc
- S procs: ditto (at same time)
- R procs: find cell/cell overlaps, perform interpolation
- R procs: send final results to S or T procs

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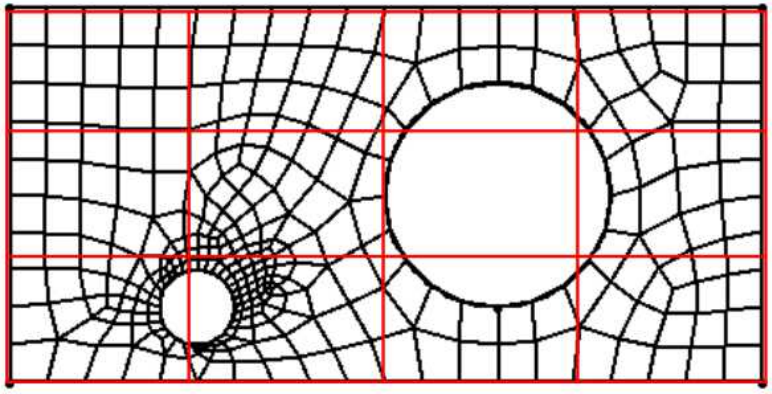

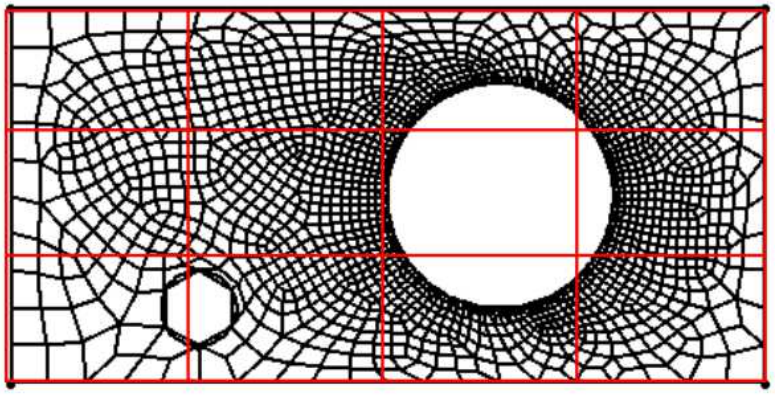

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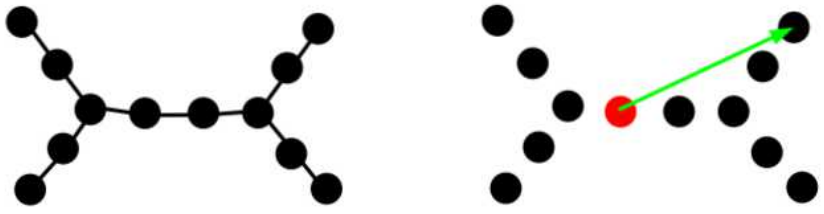
JPDC paper showed rendezvous comm can be **quite fast**

# Rigid body setup in LAMMPS

Identify central particle per body, bcast ID to other particles



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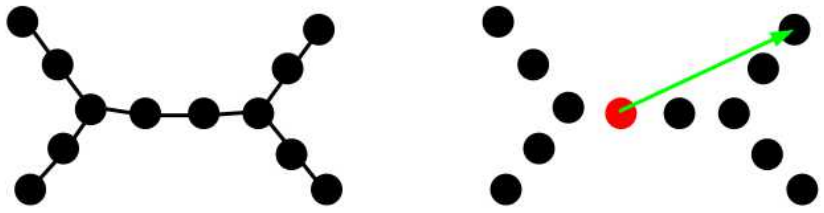


Rendezvous algorithm:

- Rvous decomp: each proc owns **random subset** of body IDs
- Send one datum per particle: particle ID, coords, proc ID
- Rvous proc receives all particles in body, computes info
- Send one datum per particle: particle ID, center particle ID

# Weak scaling results for rigid body setup

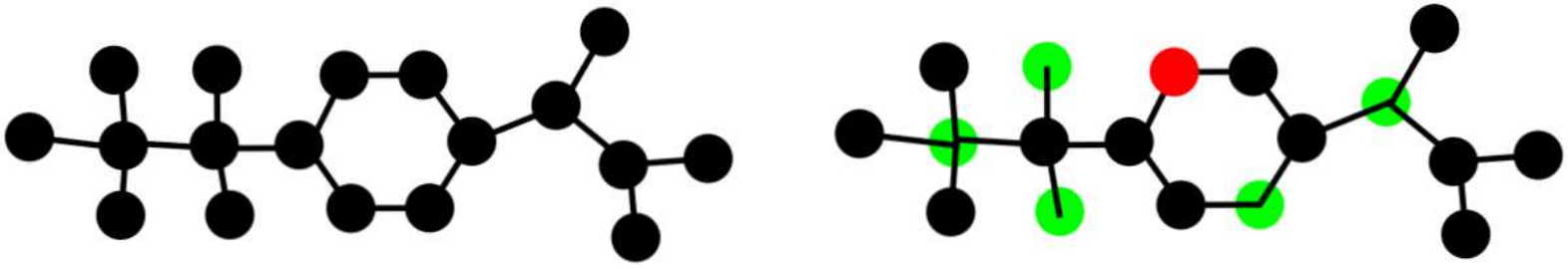
Mira BG/Q at ALCF: 1 node to 48K nodes, upto **9B** particles

| Nodes | 1 | 64 | 256 | 1K | 4K | 16K | 48K |
|---|---|---|---|---|---|---|---|
| MPI | 16 | 1K | 4K | 16K | 64K | 256K | 768K |
| Bodies | 5K | 336K | 1.3M | 5.4M | 22M | 86M | 258M |
| Atoms | 184K | 12M | 47M | 188M | 752M | 3.0B | 9.0B |
| Ring | **0.121** | 7.56 | 31.0 | 127 | 497 | *2000 | ***6000** |
| Rvous | **0.027** | 0.028 | 0.033 | 0.066 | 0.27 | 1.2 | **3.5** |

- Ring: each proc scans all the datums
- Rvous: each proc receives exactly the N/P data it needs
- Asterisk timings are estimates
- 4x to 1700x advantage for rendezvous algorithm
- Don't care on 256 nodes with 47M atoms, but do at scale

# Bond walking setup in LAMMPS

Molecules as graphs: find 1st, 2nd, 3rd, etc neighs of each atom



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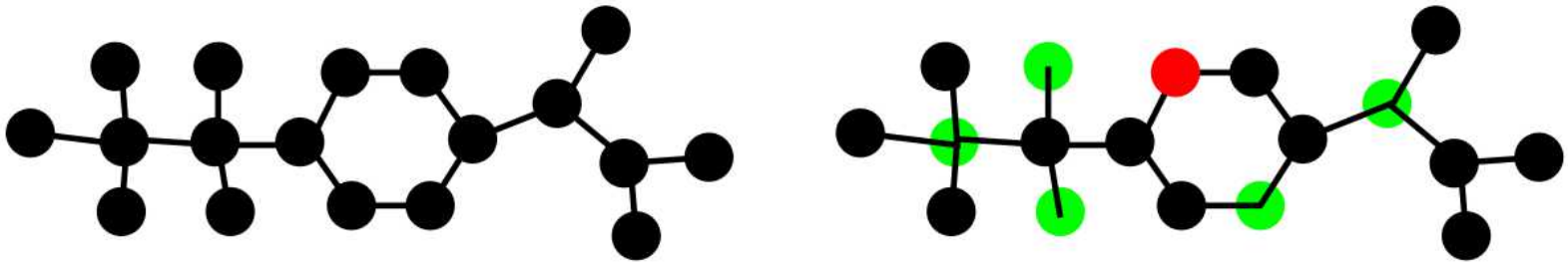


Rendezvous algorithm: **once for each level** of neighbors
Example: find 2nd neighs from 1st neighs

- Rvous decomp: each proc owns every Pth atom ID
- Send one datum (I, proc) per owned atom, to I owner
- Double loop over 1st neighbors of each atom I:
  - send **two datums** (J,K) to J owner and (K,J) to K owner
  - only comm atom pairs with a ghost atom
- Rvous proc re-sends (J,K) datums to J owner
- 3rd neighs: double loop over 1st neighs and 2nd neighs

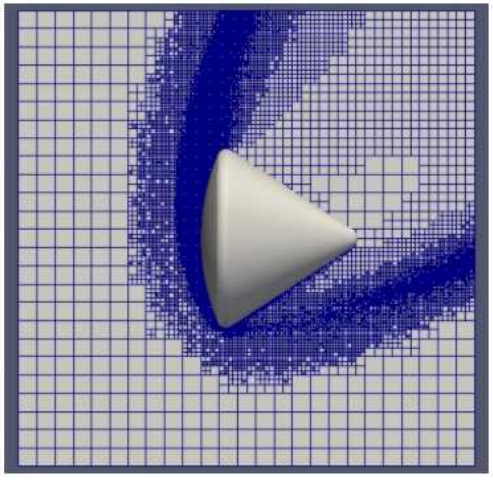
# Weak scaling results for bond walking setup

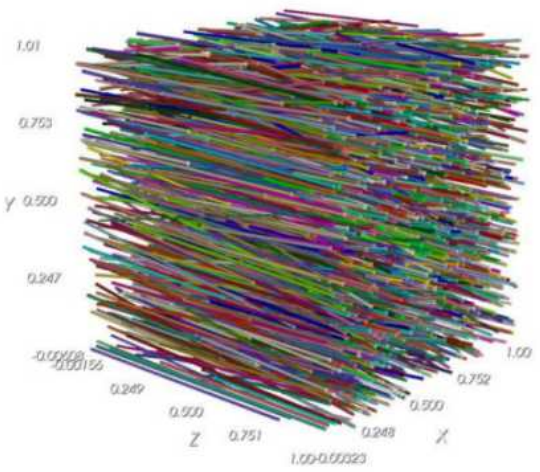
Mira BG/Q at ALCF: 64 nodes to 48K nodes, upto **37B** atoms

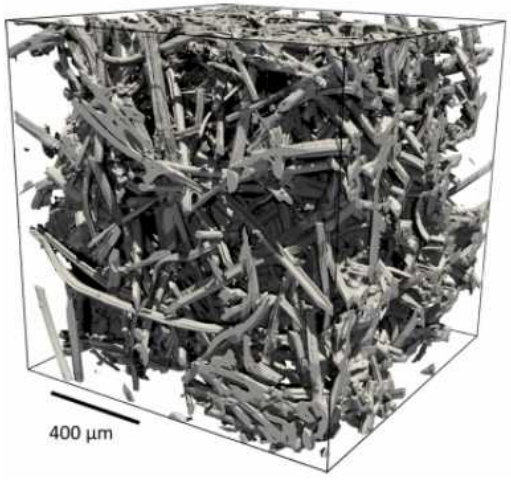
| Nodes | 64 | 256 | 1K | 4K | 16K | 32K | 48K |
|---|---|---|---|---|---|---|---|
| MPI | 1K | 4K | 16K | 64K | 256K | 512K | 768K |
| Atoms | 48M | 192M | 768M | 3.1B | 12B | 25B | 37B |
| Ring | **91.5** | 366 | 1465 | *6120 | *24500 | *49000 | ***73500** |
| Rvous | **0.912** | 0.942 | 1.14 | 1.82 | 4.95 | 9.15 | **13.2** |

- Again, asterisk timings are estimates
- 100x to 5000x advantage for rendezvous algorithm

# Surface element to grid cell mapping in SPARTA (DSMC)






- Hierarchical grid, triangulated surfaces
- Each proc owns cluster of grid cells
- Each grid cell needs list of intersecting surface elements

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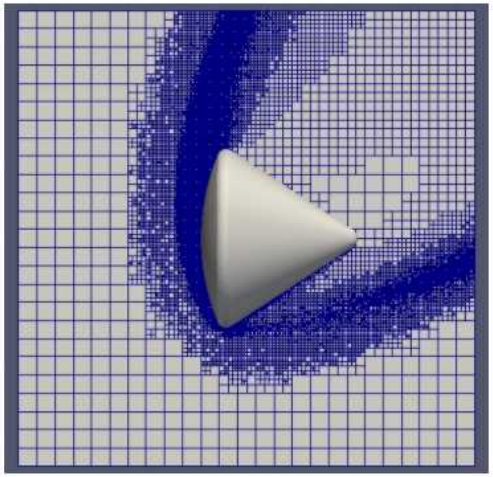

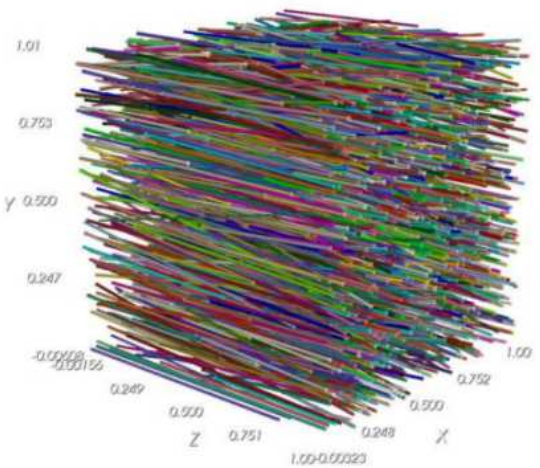



- Hierarchical grid, triangulated surfaces
- Each proc owns cluster of grid cells
- Each grid cell needs list of intersecting surface elements
- For small triangle counts:

  faster to let each grid cell check all surfs
- For huge triangle counts: **faster to flip it**
  - each proc loops over N/P surfs
  - for each surf, identify grid cells in bounding box
  - create list of grid cells that intersect each surf
  - **But**: results are stored opposite of how needed

# Rendezvous converts cells-per-surf to surfs-per-cell

- Rvous decomp: each proc owns **random subset** of grid IDs
- Send one datum per owned grid cell: grid ID, proc ID
- Send one datum per intersection: grid ID, triangle ID
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| Nodes | 64 | 64 | 256 | 256 | 1K | 1K | 4K | 16K |
|---|---|---|---|---|---|---|---|---|
| MPI | 1K | 1K | 4K | 4K | 16K | 16K | 64K | 256K |
| Surfs | 1.3M | 1.3M | 1.3M | 1.3M | 1.3M | **2M** | 1.3M | 1.3M |
| GCells | 1M | 8M | 8M | 64M | 1M | 128M | 64M | 256M |
| Old | **105** | 813 | 204 | 1600 | 104 | **1260** | 104 | 105 |
| Rvous | **3.2** | 3.5 | 3.0 | 3.3 | 2.7 | **7.5** | 2.9 | 3.9 |

- 1.3M or 2M triangles, vary grid cells and nodes
- 33x to 170x advantage for new inverted algorithm
- Rendezvous comm itself is small fraction of total

# Black-box implemention of rendezvous communication

rvous (N_in, indata, sendprocs1, callback()):

N_rvous = **MPI_All2allv**() of indata ⇒ indata_rvous

**callback**(N_rvous,indata_rvous,outdata_rvous,sendprocs2)

N_out = **MPI_All2all**() of outdata_rvous ⇒ outdata

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- 2 All2all comm ops, sandwiching a callback to process data
- Callback allows each proc to compute on Rvous data
- Can use **irregular** comm operation instead
- Irregular is faster if each proc sends to a few procs
- All2all is faster if each proc sends to (nearly) all procs

# One more communication pattern

MapReduce - from Google and 


- MapReduce is not just for data, also for scientific computing
- A mapper reads/creates datums and sends them to reducers

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MapReduce lib on top of MPI: **http://mapreduce.sandia.gov**
We used it for graph algorithms: e.g. connected components

# Conclusions

**Attributes** of rendezvous algorithms:

- Useful when don't know how to move data where needed
- Can auto-load-balance if randomly spread the data
- Leverages huge bisection message bandwidth of big computers
- Someone paid for it, why not use it !

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- Better to load balance individual stages of a computation
- Pay the extra cost for comm in between
- Rather than perform all stages with poor load-balancing

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What about **GPUs** ?

- There are no more machines with 1M+ MPI tasks
- Still useful at scale for ops that don't map to GPUs
- Occasional ops: setup, rebalance, grid-adaptation, etc