Distributed Parallel Methods in Psi4

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Psi 4 Developer's Meeting
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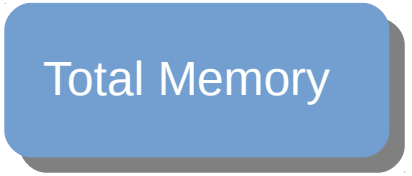
Distributed vs. Shared Memory



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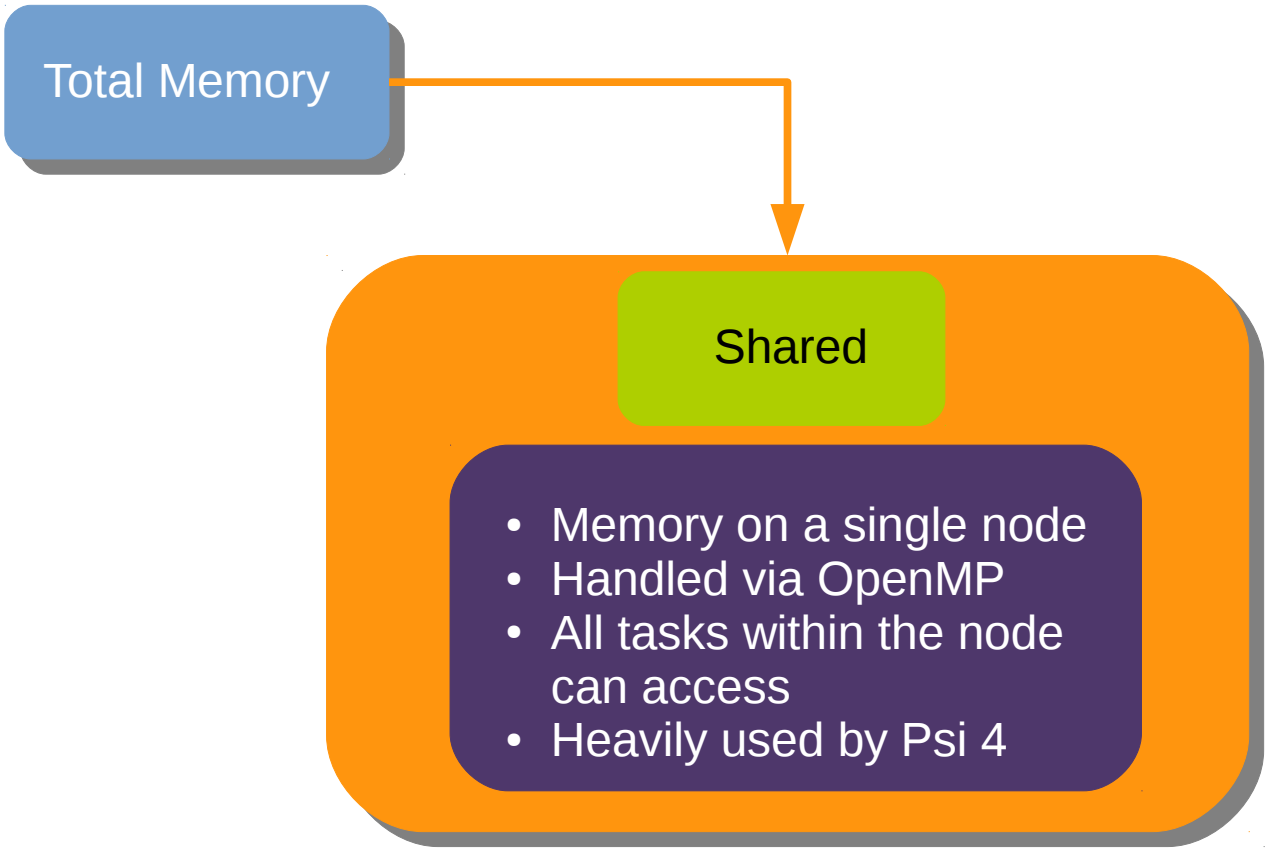

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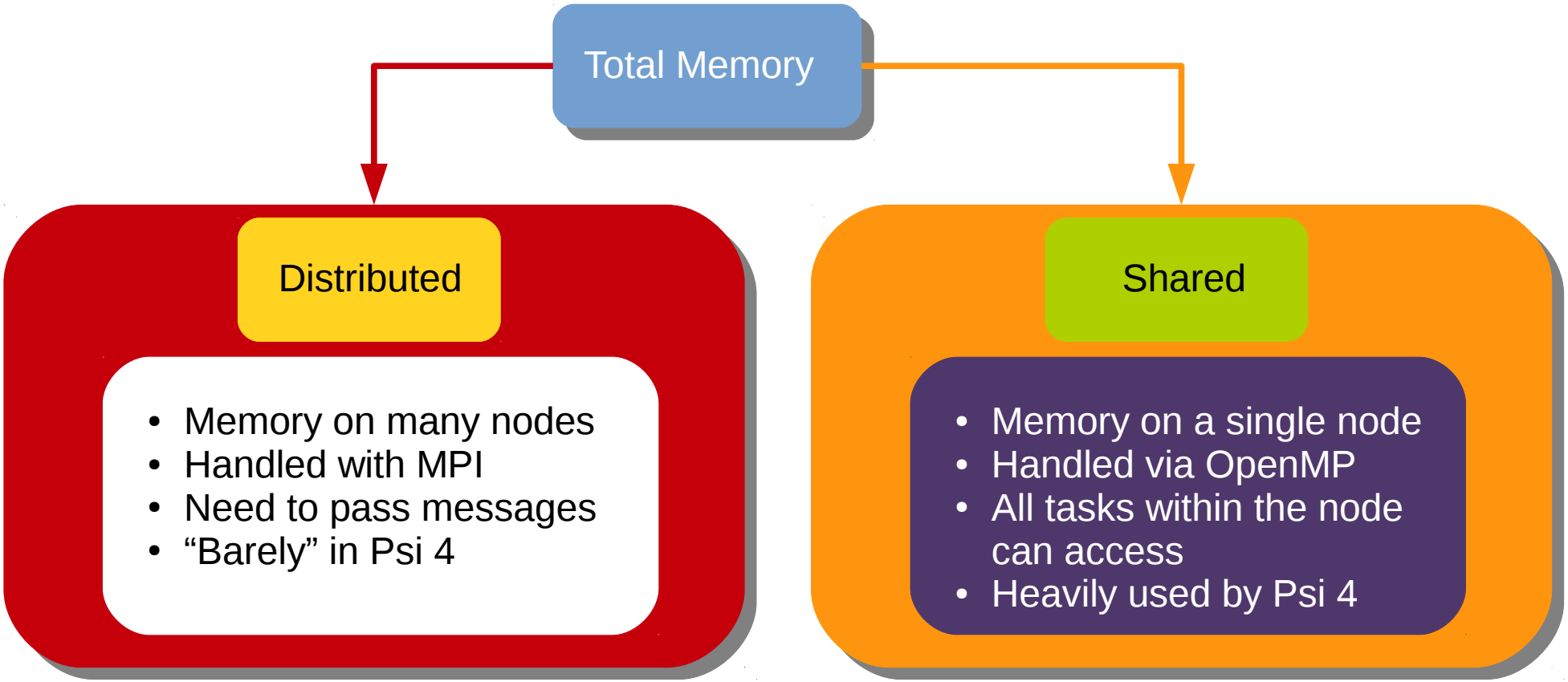

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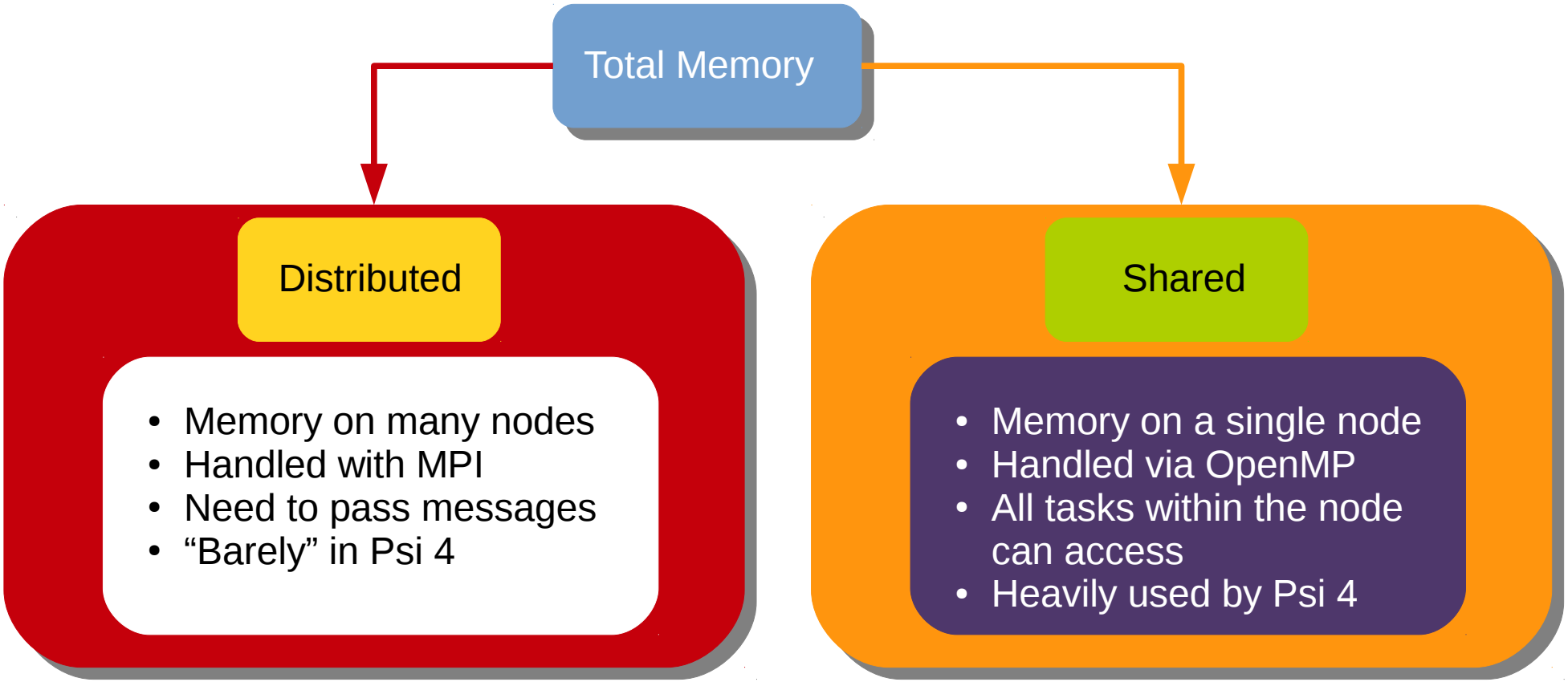


All my projects relate to introducing MPI
Into Psi 4

GTFock Interface: LibJKFactory

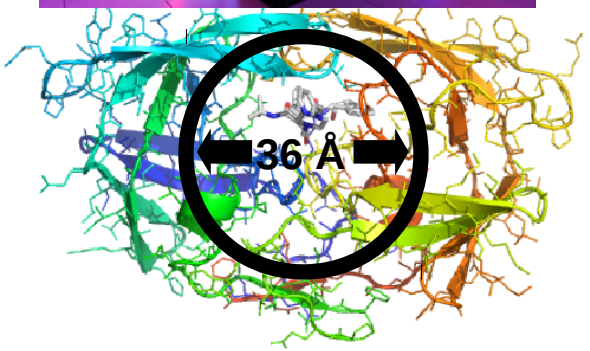
- Designed to compute J and K matrices
  - Uses:
    - MPI
    - MKL
    - Global Arrays
    - Modified ERD
- Demonstrated scaling to 156,000 cores
  - Tianhe-2
- Intended to be used throughout:
  - HF
  - DFT
  - SAPT

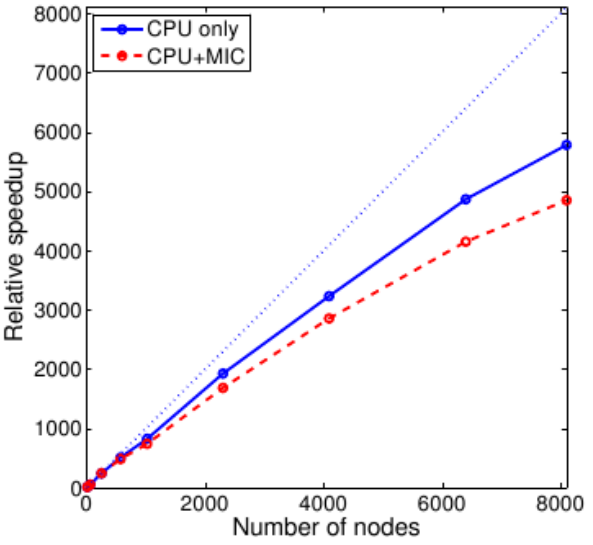
Collaboration with:

Edmond Chow

Xing Liu

School of Computational Science and Engineering at GT





GTFock Interface: LibJKFactory

- Status:
  - Working with spherical basis sets
    - Normalization issue with Cartesian
  - Timings underway
    - OptERD vs. LibInt
    - Cost of scatter/gather

LibFrag

Generalized Many Body Expansion (MBE)

$$E \approx \mathcal{E}^{(1)} + \Delta\mathcal{E}^{(2)} + \cdots + \Delta\mathcal{E}^{(n)}$$

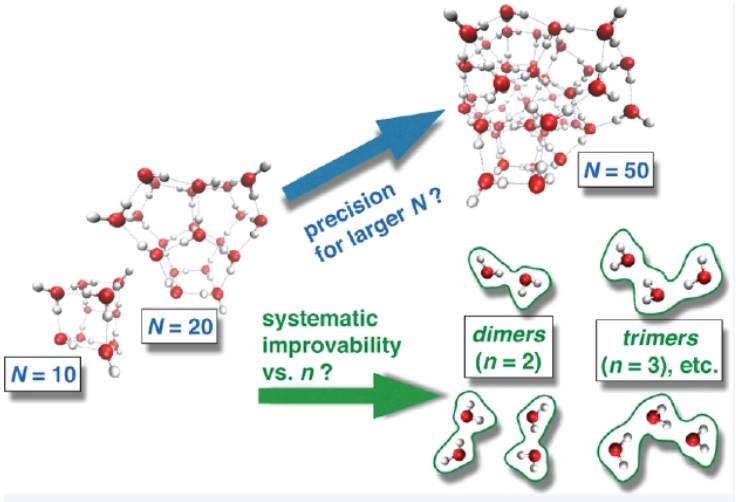
$$\Delta\mathcal{E}^{(n)} = \mathcal{E}^{(n)} - \mathcal{E}^{(n-1)}$$

$$\mathcal{E}^{(n)} = \sum_{I=1}^{\binom{N}{n}} E_I^{(n)} - \sum_{I=1}^{\binom{N}{n}} \sum_{J>I}^{\binom{N}{n}} E_{I\cap J}^{(n)} + \cdots + (-1)^{\binom{N}{n}+1} E^{(n)}_{I\cap J\cap\cdots\cap\binom{N}{n}}$$

Reduces to MBE for disjoint fragments

$$E^{(n)} = \sum_{k=1}^{n} (-1)^{n-k} \binom{N-k-1}{n-k} \sum_{K=1}^{\binom{N}{k}} E_K^{(k)}$$

- (G)MBE super-molecular alternative to SAPT
  - Property decomposition expansion
  - Applicable to any extensive property
- GMBE is a universal energy equation
  - Can put other fragment methods in terms of it
  - Basis of current library



Shameless self-promotion:
Richard, Lao, Herbert. Acc. Chem. Res. 47 (2014) 2828-2836.

LibFrag

- Distinguishing components of a fragment method:
  - How are the fragments formed?
  - How are severed bonds dealt with?
  - How are orders > n accounted for?
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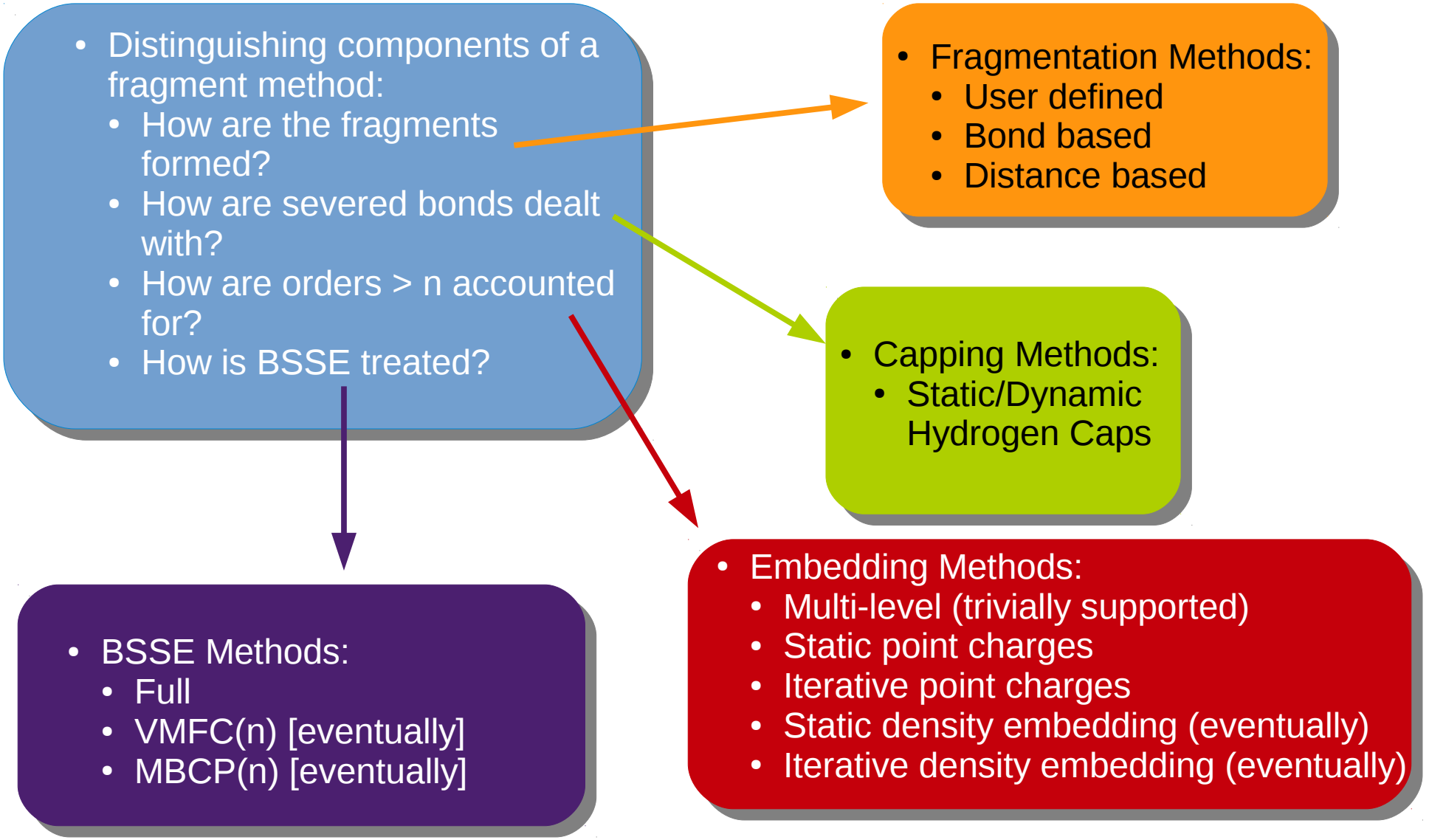
- Embedding Methods:
  - Multi-level (trivially supported)
  - Static point charges
  - Iterative point charges
  - Static density embedding (eventually)
  - Iterative density embedding (eventually)

LibFrag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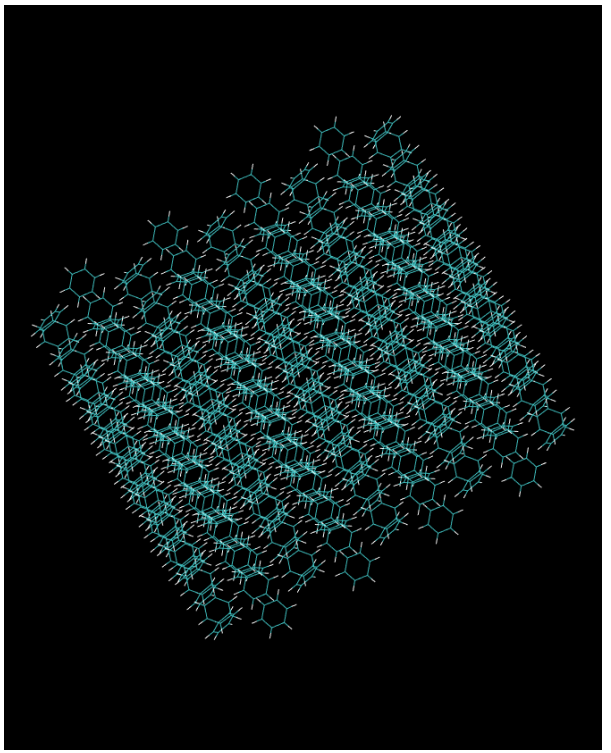
Embedding Methods:
Multi-level (trivially supported)
Static point charges
Iterative point charges
Static density embedding (eventually)
Iterative density embedding (eventually)
BSSE Methods:
Full
VMFC(n) [eventually]
MBCP(n) [eventually]

LibFrag

- Highlights:
  - Hybrid MPI/OpenMP
  - Flexible and extensible
  - Highly automated
  - Re-use of SCF guesses
  - Capable of handling very large systems (~5,000 atoms)
  - Space group symmetry exploiting
  - Capable of creating periodic systems from unit cells



MPI Utilities

- Goal: Provide a universal, simple interface to Psi 4's MPI Capabilities
- Automatically:
  - Handles data synchronization
  - Load balancing
  - Communicator allocation

- Plans for:
  - Python Interface
  - Dynamic addition of tasks
  - Prolonged proliferation of distributed data

- As far as user is concerned:
  - MPITask Class
    - Holds details of what you want to parallelize
  - MPIJob Class
    - Gives you your instructions

MPI Utilities

- Label: input for a job. Purely for your convenience
- Could be:
  - Shell quartet for integrals
  - Element number for vector addition
  - Calculation name for databases
  - Atom and component for finite difference

```
//Declare an array of Tasks, with labels of type
//T.  T can be anything that is convenient for you
std::vector<MPITask<T> > MyTasks;
for (int task=0; task<NTasks; ++task){
      T Label=GetLabel(task);//Get this task's label
      int Priority=GetPriority(task);//Get this task's priority
}

MPIJob<T> Job(MyTasks);//Make a job manager

std::vector<T2> Data;//Our generated data, of type T2

for(T task=Job.Begin(); !Job.Done(); task=Job.Next())
   Data.push_back(NewData(task)); //Collect the data

//Give everyone a copy of the data point
std::vector<T2> AllData=Job.Synch(Data,1);

//Multiply all the data together and return a value
T2 product=Job.Reduce(Data,1,MULTIPLY);
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A more advanced Job interface exists for those who know MPI and want to Avoid scatter/gathers

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Acknowledgments

- Sherrill Group
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- Georgia Tech
- NSF

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