MPI-QUICK

Yipu Miao
University of Florida

WHAT IS QUICK?

- **Quick is a linear scaling ab initio and density functional theory program. Featured with:**
  - **Linear scaling Divide and Conquer (D&C)**
  - **Single point ab initio and DFT**
  - **Geometry Optimization**

- for calculation of energies, charges and geometries of systems up to ~3,000 atoms. Available features include

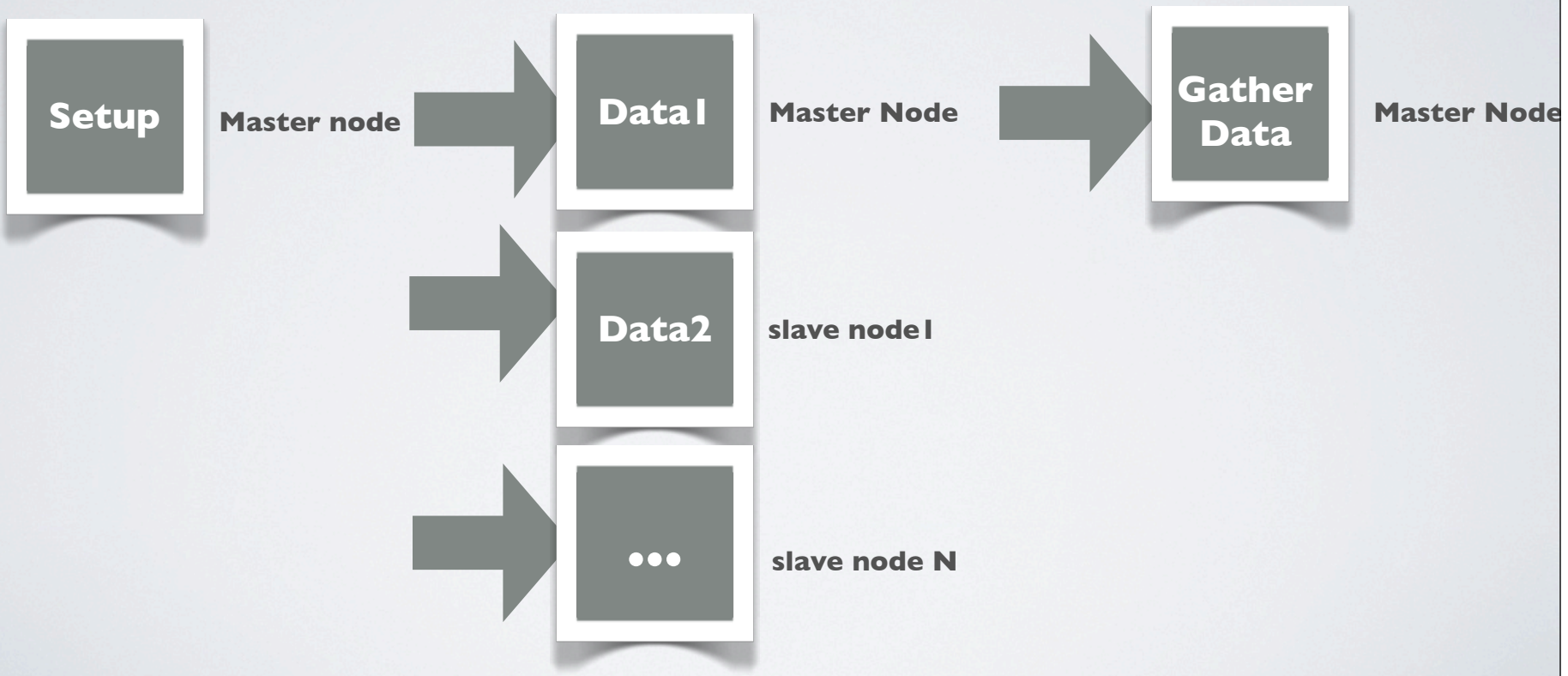
Development history:
Ed Brothers: Basic
Ken Ayers and Xiao He: optimized the code.

MPI

- **MPI - Message Passing Interface**
- **C/C++/F77/F90 Bindings**
- **Distributed Memory Programming**
- **Series of Function**

Single Node

MPI



A.HARTREE-FOCK

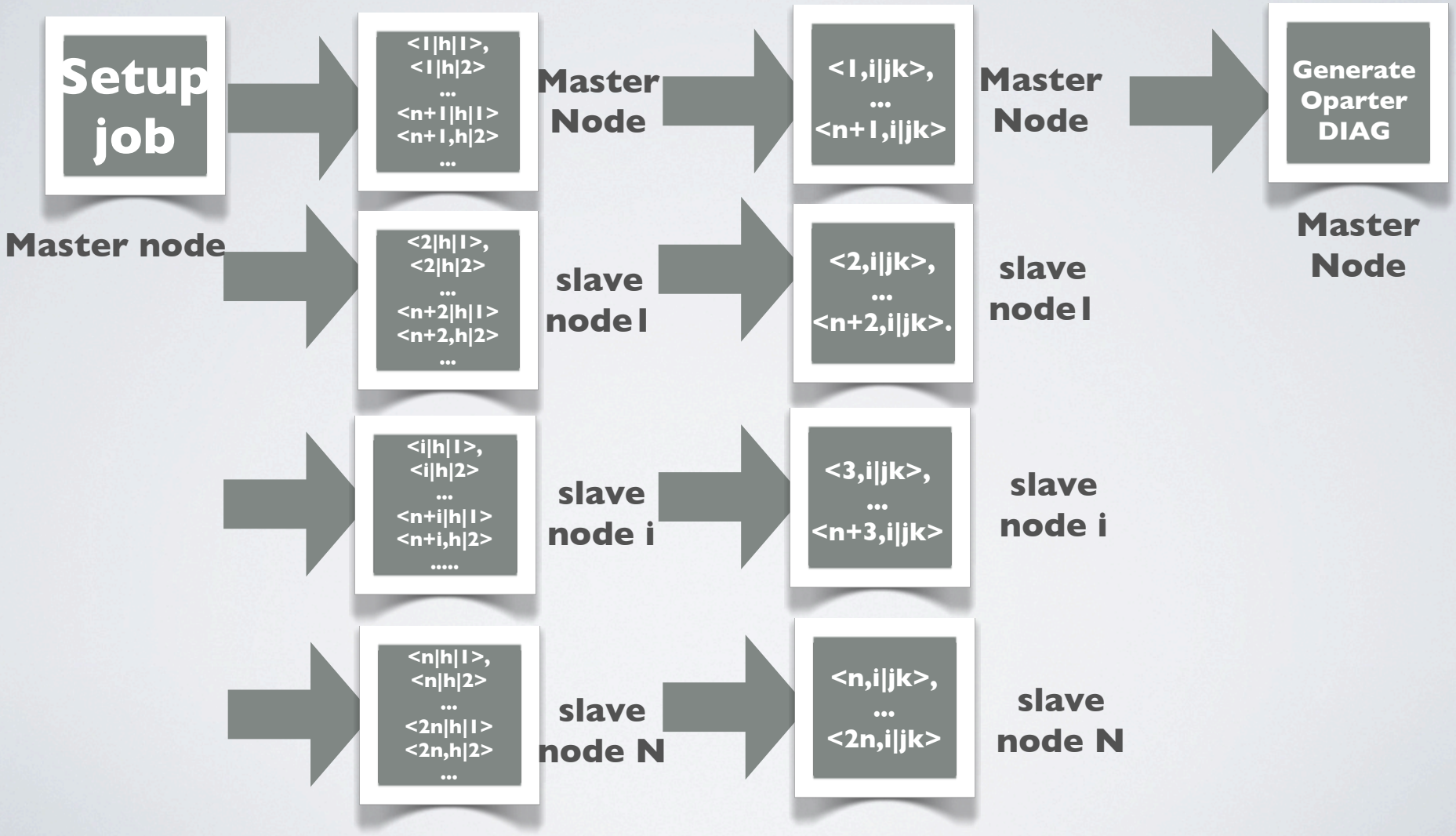
$$\langle i|h|j\rangle = \int d\mathbf{x}_1 \chi_i^*(\mathbf{x}_1) h(\mathbf{r}_1) \chi_j(\mathbf{x}_1)$$

$$[ij|kl] = \int d\mathbf{x}_1 d\mathbf{x}_2 \chi_i^*(\mathbf{x}_1) \chi_j(\mathbf{x}_1) \frac{1}{r_{12}} \chi_k^*(\mathbf{x}_2) \chi_l(\mathbf{x}_2).$$

$$\mathbf{FC} = \mathbf{SC}\epsilon$$

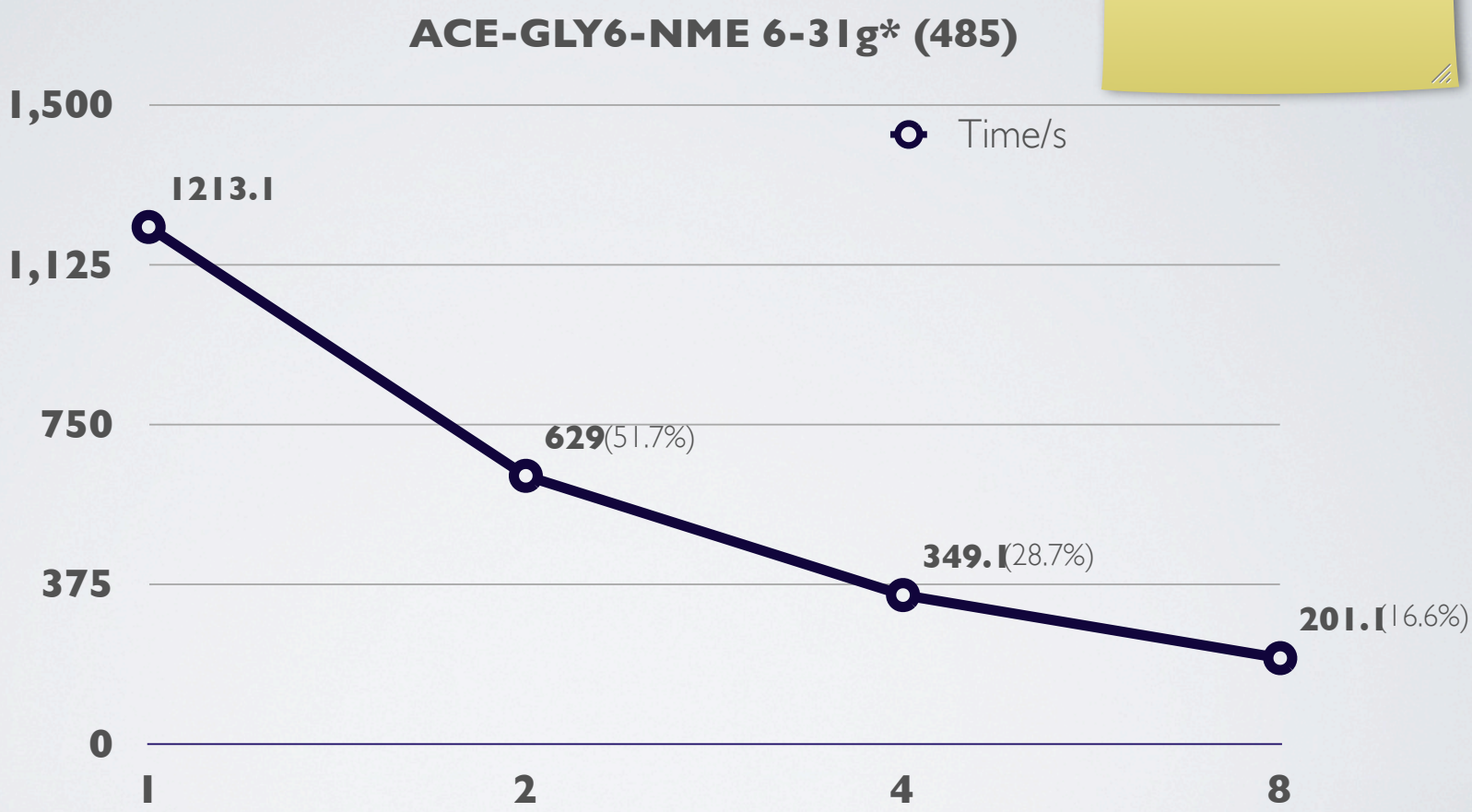
$$E_{HF} = \sum_i \langle i|h|i\rangle + \frac{1}{2}\sum_{ij}[ii|jj] - [ij|ji],$$

FLOWCHART FOR HF



HF PARALLEL

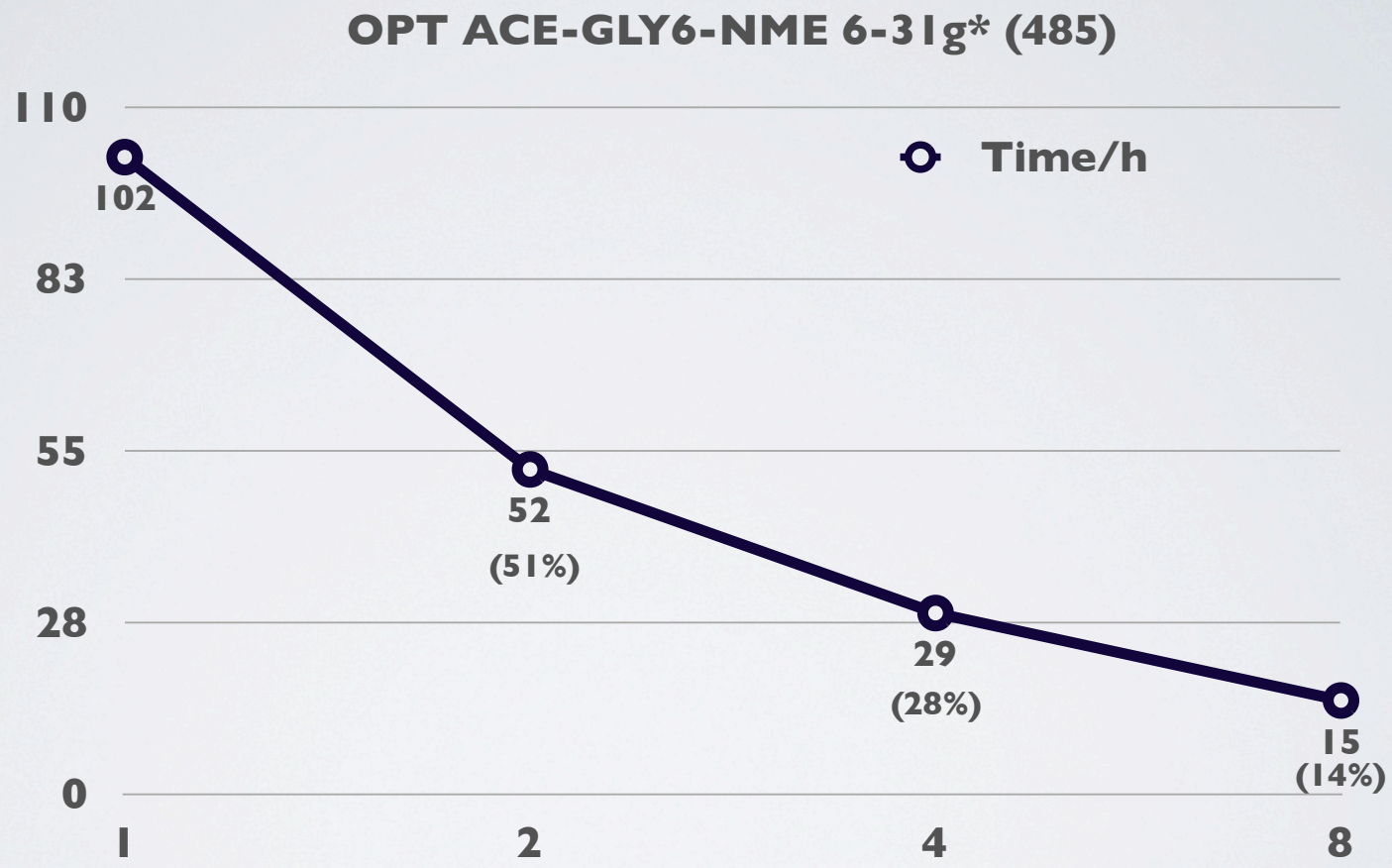
Acetic-Glycine6

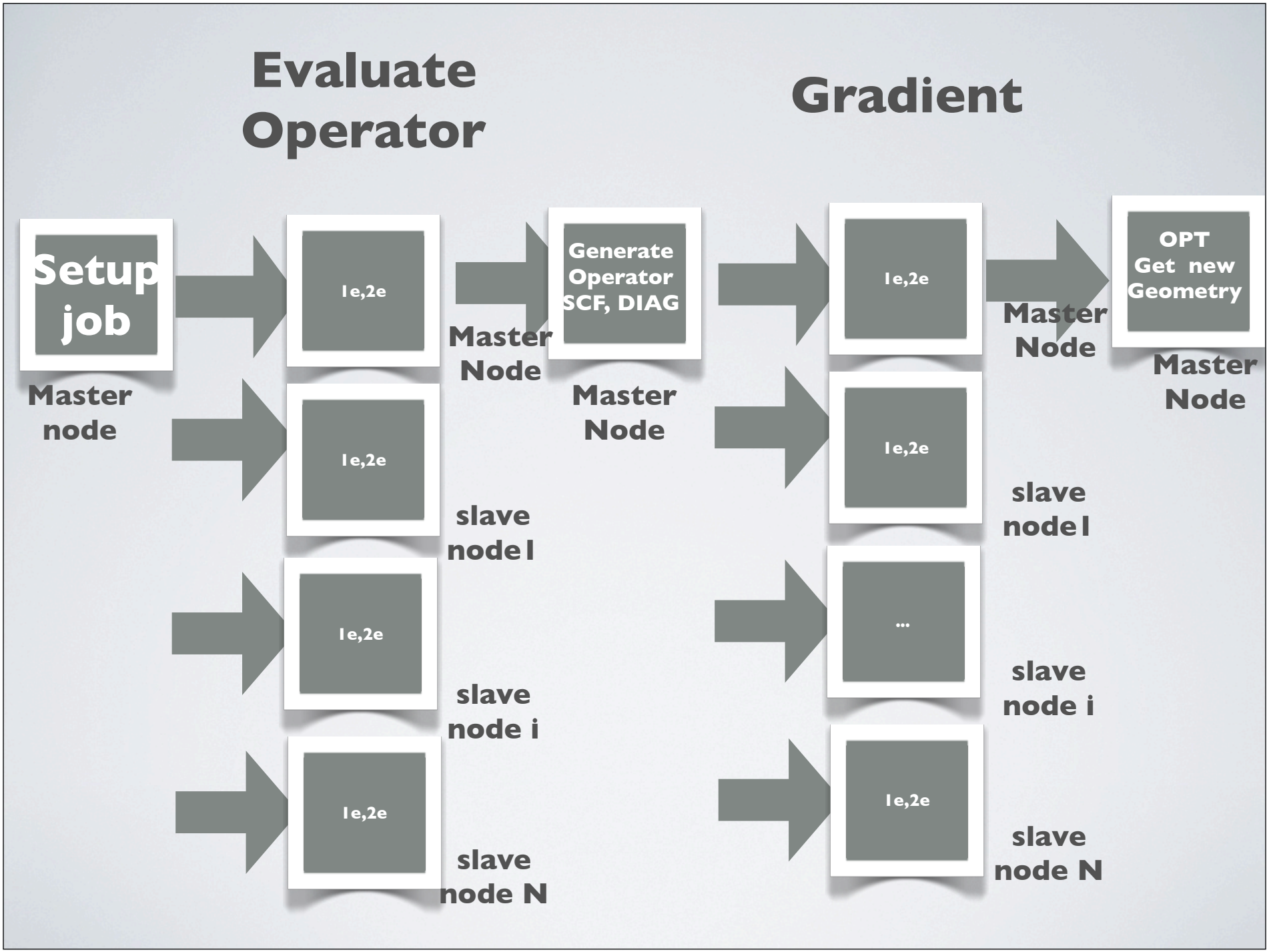


BREAK DOWN

	1	2	4	8
1e	4.14	2.11 (51%)	1.09 (26%)	0.51 (12%)
2e	1171	588 (50%)	267 (23%)	143 (12%)
Operator	1202	620 (52%)	309 (26%)	194 (16%)
Total CPU time &	1213	1217 (99.6)	1244 (97.5%)	1220 (99.4%)

B.HF OPT PARALLEL

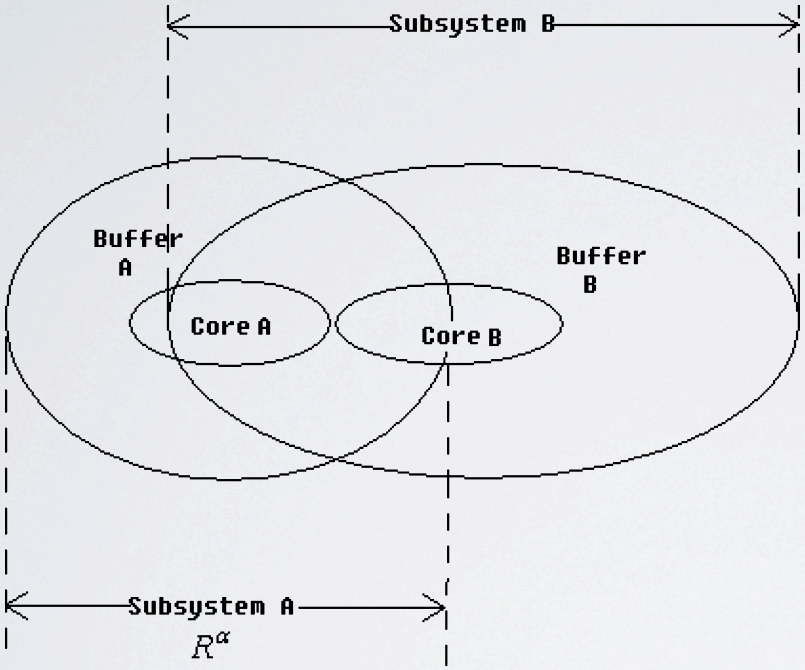



Evaluate Operator
Gradient
Setup job
Master node
1e,2e
1e,2e
1e,2e
1e,2e
slave node I
slave node i
slave node N
Master Node
Generate Operator SCF, DIAG
Master Node
1e,2e
1e,2e
...
1e,2e
Master Node
slave node I
slave node i
slave node N
OPT Get new Geometry
Master Node

BREAK DOWN

	1	2	4	8
1e	723	365 (51%)	187 (26%)	90.6 (12.5%)
2e	125812	62384 (50%)	28524 (23%)	15651 (12.4%)
Operator	126812	63630 (50%)	33621 (26%)	17801 (14%)
Gradient	183863	90916 (49%)	41582 (23%)	22930 (12.5%)
Total CPU time & Eff	313234	316645 (98.9%)	331017 (94.6%)	317692 (98.6%)

C.DIVIDE-AND-CONQUER HF

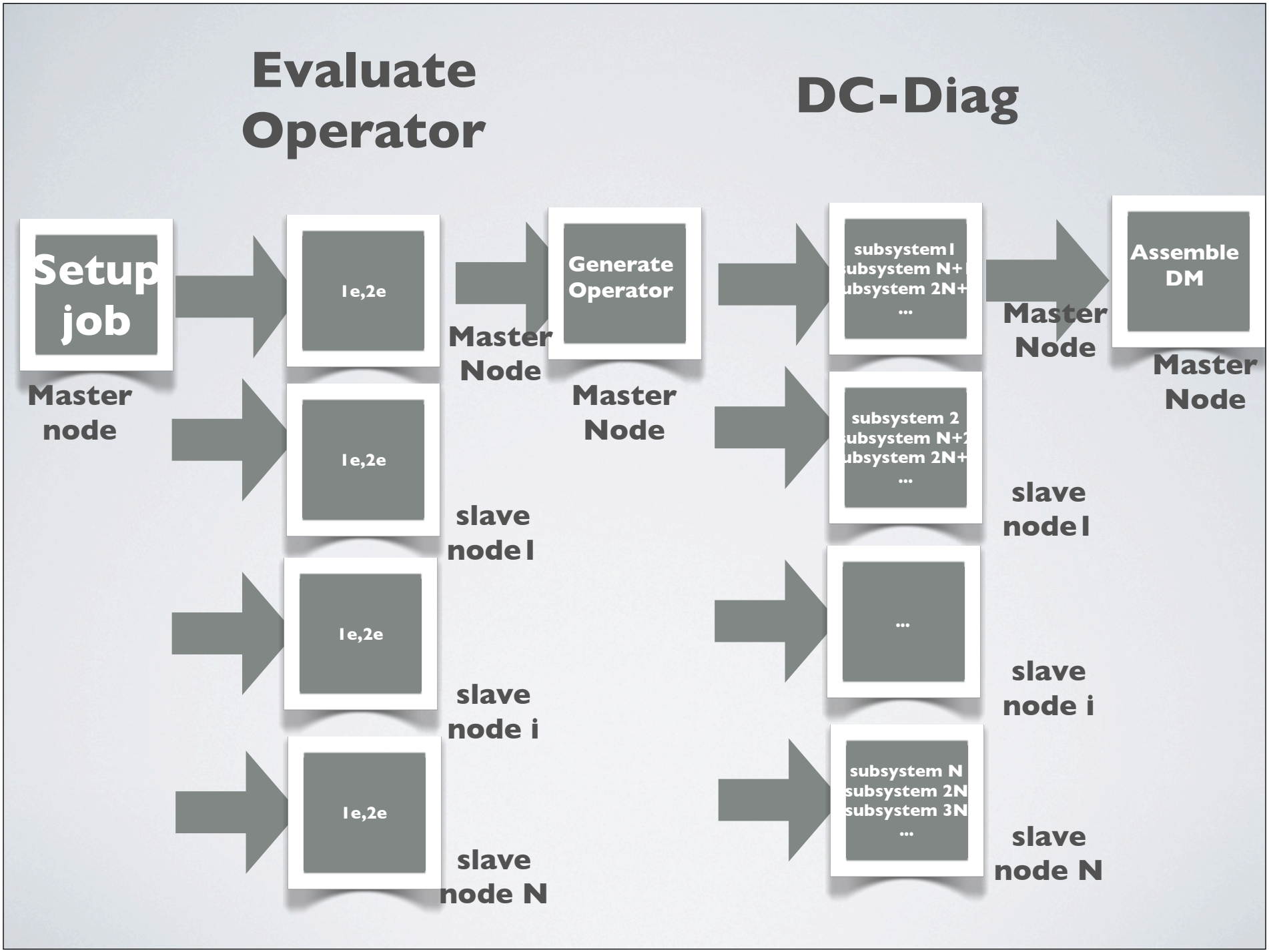


$$F^\alpha C^\alpha = S^\alpha C^\alpha E^\alpha$$

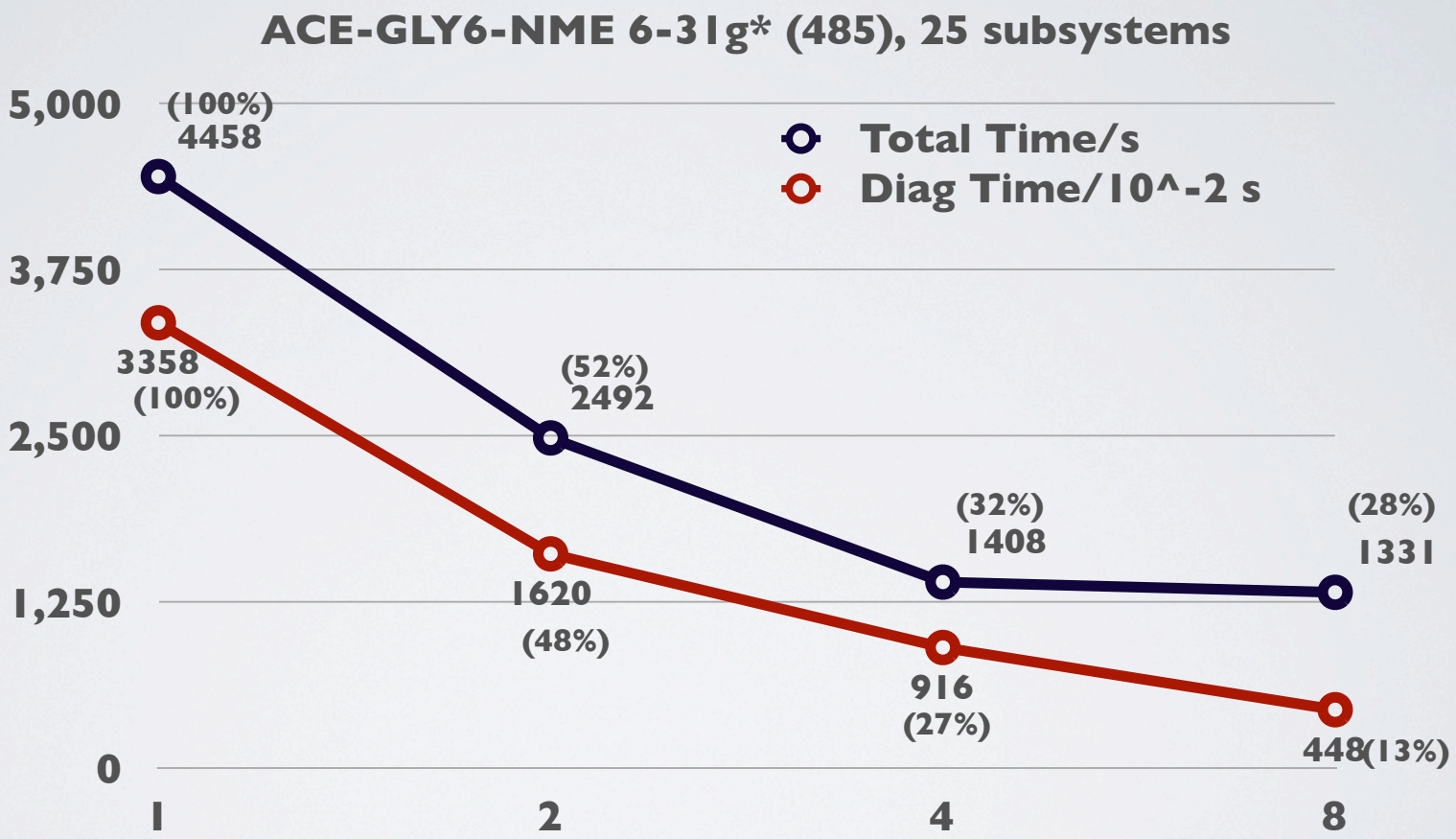
$$F^\alpha_{\mu\nu} = \begin{cases} F_{\mu\nu} \text{ if } \chi_\mu \in R^\alpha \text{ and } \chi_\nu \in R^\alpha \\ 0 \text{ elsewhere} \end{cases}$$

$$P_{\mu\nu} = \sum_{\alpha=1}^{N_{\text{sub}}} P^\alpha_{\mu\nu} = \sum_{\alpha=1}^{N_{\text{sub}}} D^\alpha_{\mu\nu} p^\alpha_{\mu\nu}$$

$$D^\alpha_{\mu\nu} = \begin{cases} 1 & \phi_\mu \in \text{Core}^\alpha \text{ and } \phi_\nu \in \text{Core}^\alpha \\ {}^1/_2 & \phi_\mu \in \text{Core}^\alpha \text{ and } \phi_\nu \in \text{Buffer}^\alpha \text{ or} \\ & \phi_\mu \in \text{Buffer}^\alpha \text{ and } \phi_\nu \in \text{Core}^\alpha \\ 0 & \phi_\mu \notin \text{Core}^\alpha \text{ and } \phi_\nu \notin \text{Core}^\alpha \end{cases}$$


Evaluate Operator
DC-Diag
Setup job
Master node
1e,2e
1e,2e
1e,2e
1e,2e
Master Node
slave node 1
slave node i
slave node N
Generate Operator
Master Node
subsystem 1
subsystem N+1
subsystem 2N+1
...
subsystem 2
subsystem N+2
subsystem 2N+2
...
...
subsystem N
subsystem 2N
subsystem 3N
...
Master Node
slave node 1
slave node i
slave node N
Assemble DM
Master Node

DIVIDE-AND-CONQUER HF PARALLEL

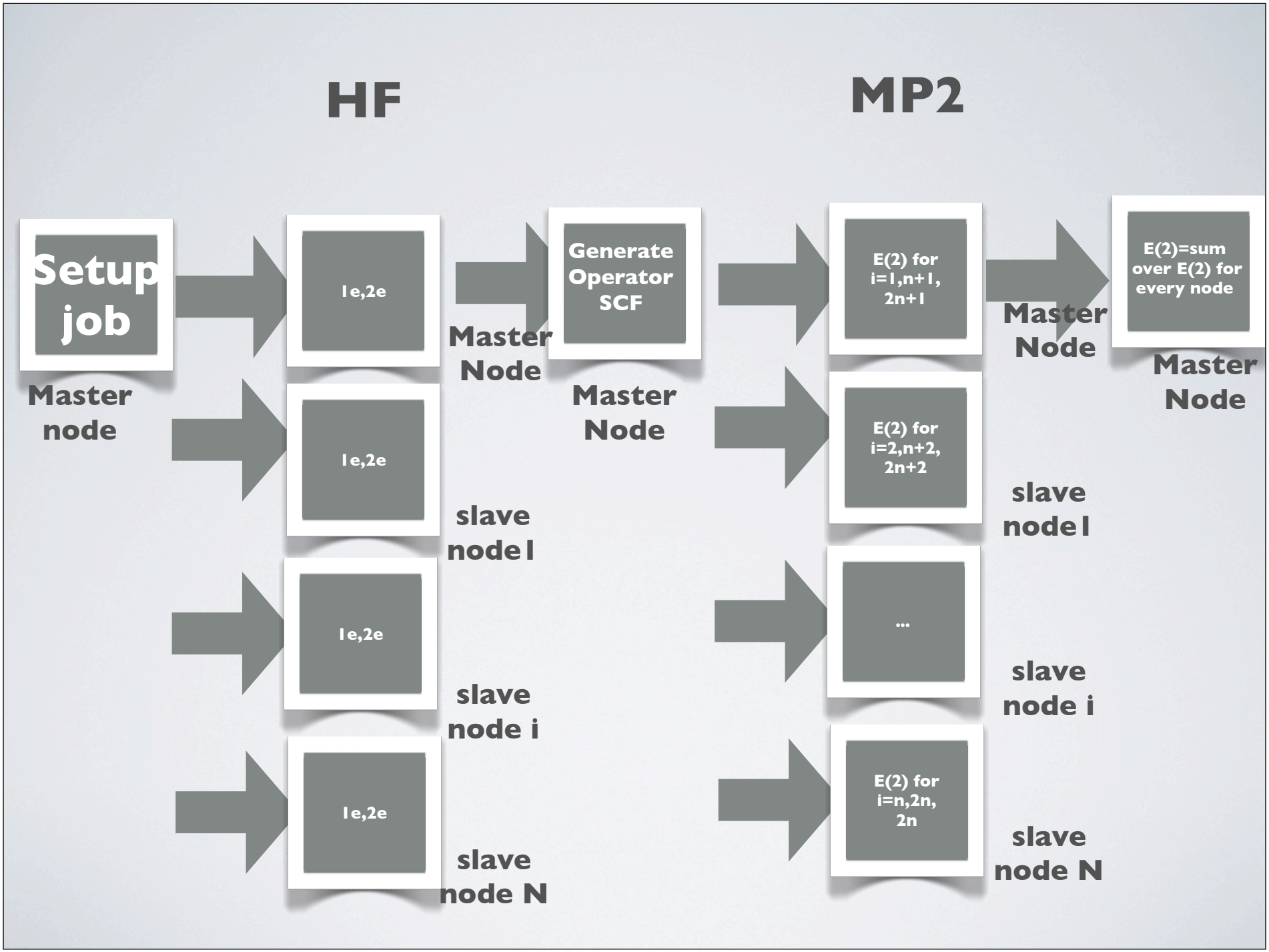


BREAK DOWN

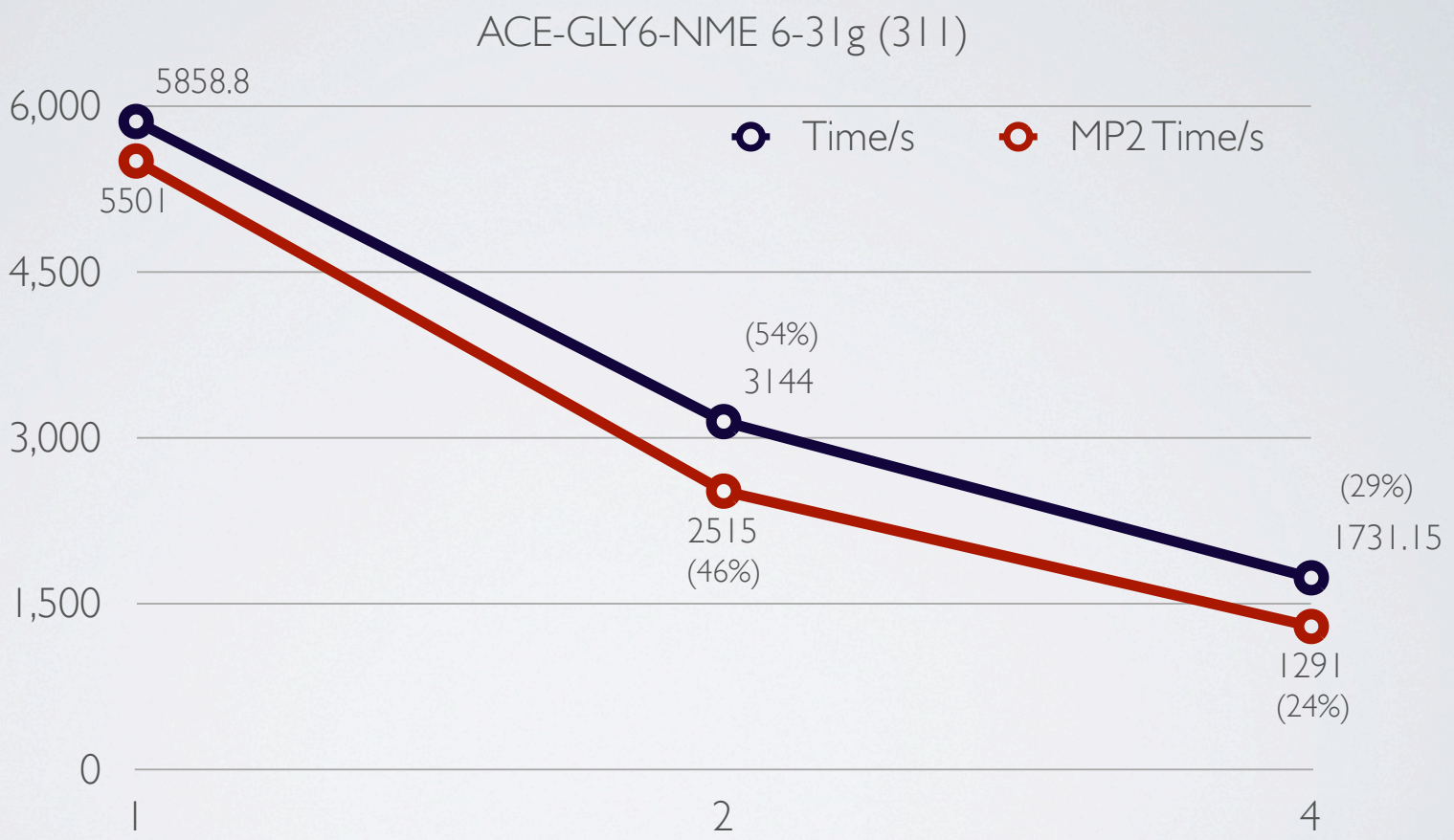
	1	2	4	8
1e	4.11	2.08 (51%)	1.08 (26%)	0.51 (12.5%)
2e	4136	2033 (49%)	935 (23%)	590 (14%)
Operator	4140	2261 (55%)	1184 (28%)	715 (17%)
Diag	33.6	16.27 (48%)	9.16 (27%)	4.48 (13%)
Total CPU time & Eff	4458	4596 (97.0%)	4627 (96.5%)	5318 (83.8%)

D. MP2 PARALLEL

$$E^{(2)} = \sum_{ijab} \frac{(ia|jb)^2 + \frac{1}{2}[(ia|jb) - (ib|ja)]^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$


HF
MP2
Setup job
Master node
1e,2e
1e,2e
1e,2e
1e,2e
slave node 1
slave node i
slave node N
Master Node
Generate Operator SCF
Master Node
E(2) for i=1,n+1, 2n+1
E(2) for i=2,n+2, 2n+2
...
E(2) for i=n,2n, 2n
slave node 1
slave node i
slave node N
Master Node
E(2)=sum over E(2) for every node
Master Node

MP2 PARALLEL



FUTURE

- DC-MP2
- Frequency
- DFT
- Integration with AMBER

ACKNOWLEDGE

- Merz group
- Ed Brother, Ken Ayers, Xiao He and other QUICK contributor

THANK YOU