Performance benchmark results for ACES III

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Outline of the talk

- Challenges in computational chemistry
  - Larger, more complex molecules
- Results for molecules of interest
  - What can be done today?
- Challenges in high performance computing
  - Parallelism at many levels

Computational Chemistry Challenges

- Larger molecules
  - Nano structures
  - Molecular electronics
  - Polymer properties
  - Biological molecules
- More emphasis on processes
  - Reaction description rather than transition probabilities

Computational challenges

- Energies
- Gradients
- Geometry search
  - Equilibrium configuration
  - Transition states
- Vibrational frequencies
- Excited electronic states

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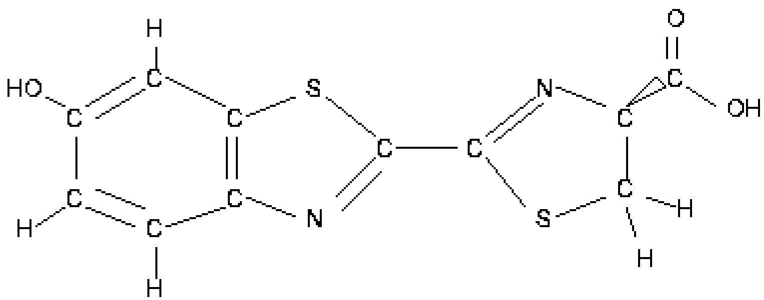
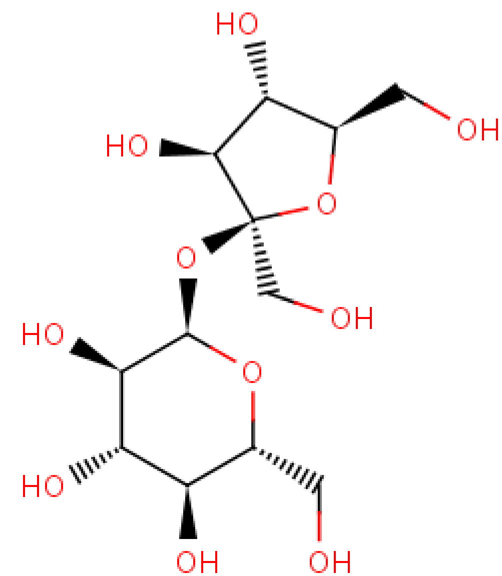
CCSD(T)

- Luciferin($C_{11}H_8O_3S_2N_2$)
- RHF
- C_1 symmetry
- Basis = aug-cc-pvdz (494 bf)
- $N^{corr}_{occc} = 46$



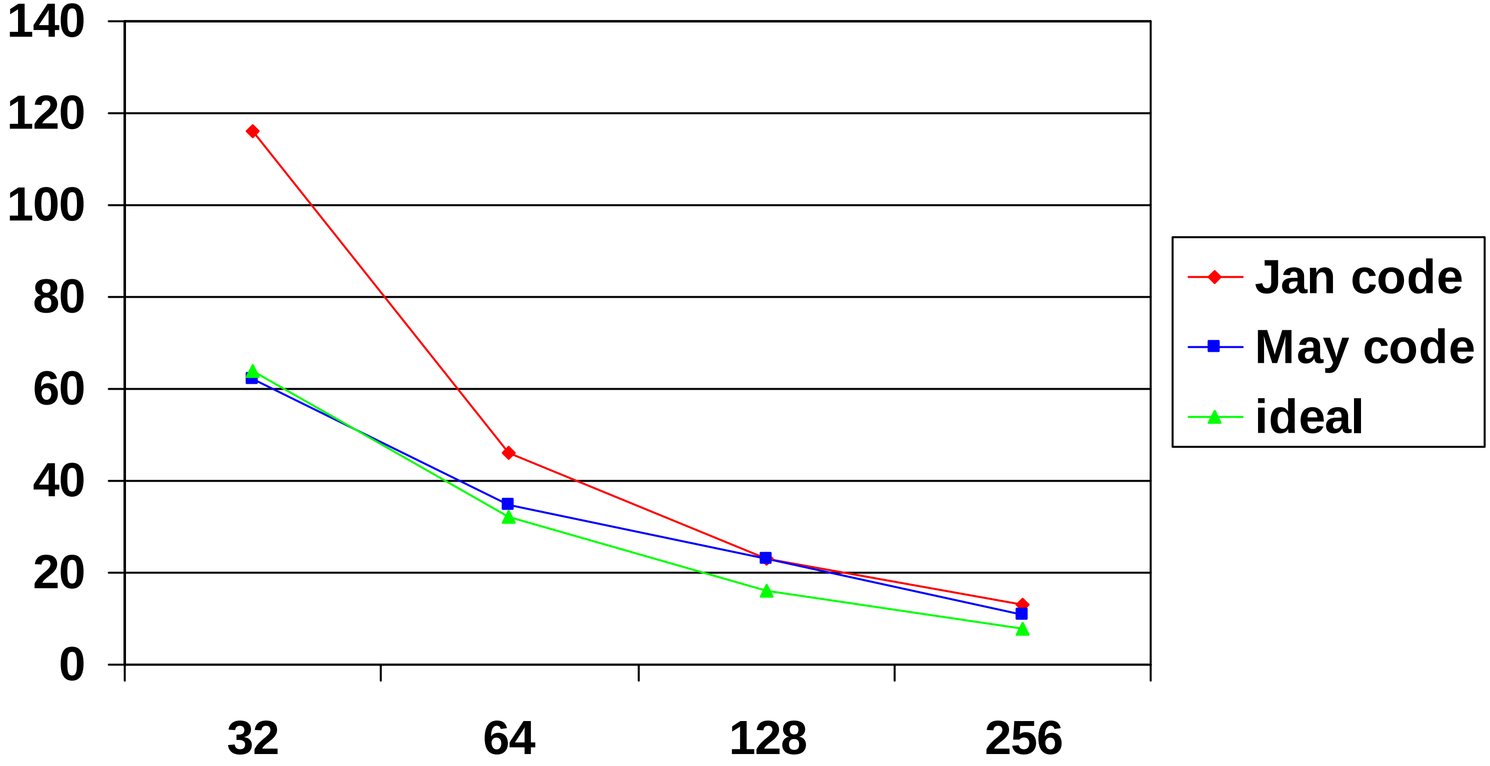
- Sucrose ($C_{12}H_{22}O_{11}$)
- RHF
- C_1 symmetry
- Basis = 6-311G** (546 bf)
- =68



ACES III software

- Developed under CHSSI CBD-03
- Parallel for shared and distributed memory
- Capabilities
  - Hartree-Fock (RHF, UHF)
  - MBPT(2) energy, gradient, hessian
  - CCSD(T) energy and gradient (DROPMO)
  - EOM-CC excited state energies

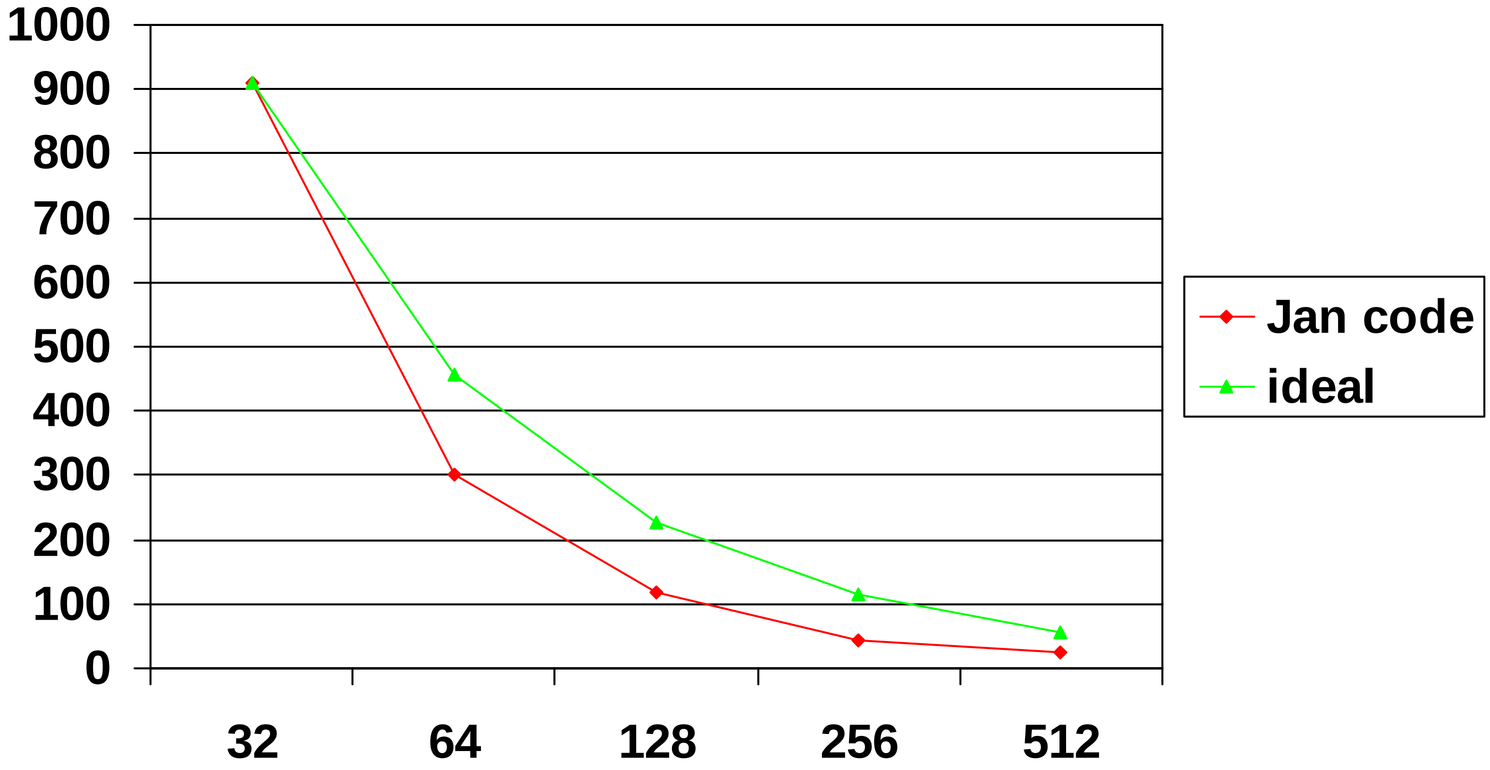
Luciferin CCSD scaling
min per iter; 12 iterations; two versions;



Luciferin CCSD(T)

- CCSD on 128 processors
  - One iteration: 23 min
  - Total 12 iterations: 275 min
- (T)
  - Hardest 8 occupied orbitals: 420 min on 128 processors
  - Total 48 correlated orbitals: 420 min on 768 processors

Sucrose CCSD scaling
min per iteration



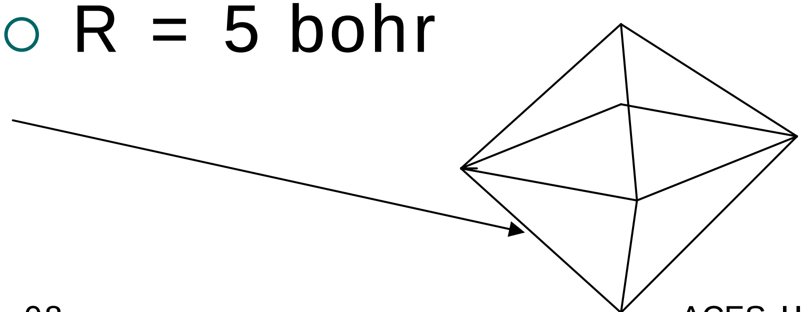
Succrose CCSD super linear scaling

- CCSD iteration
  - 32 processors 909 min
  - 512 processors 24 min, ideal: 57 min

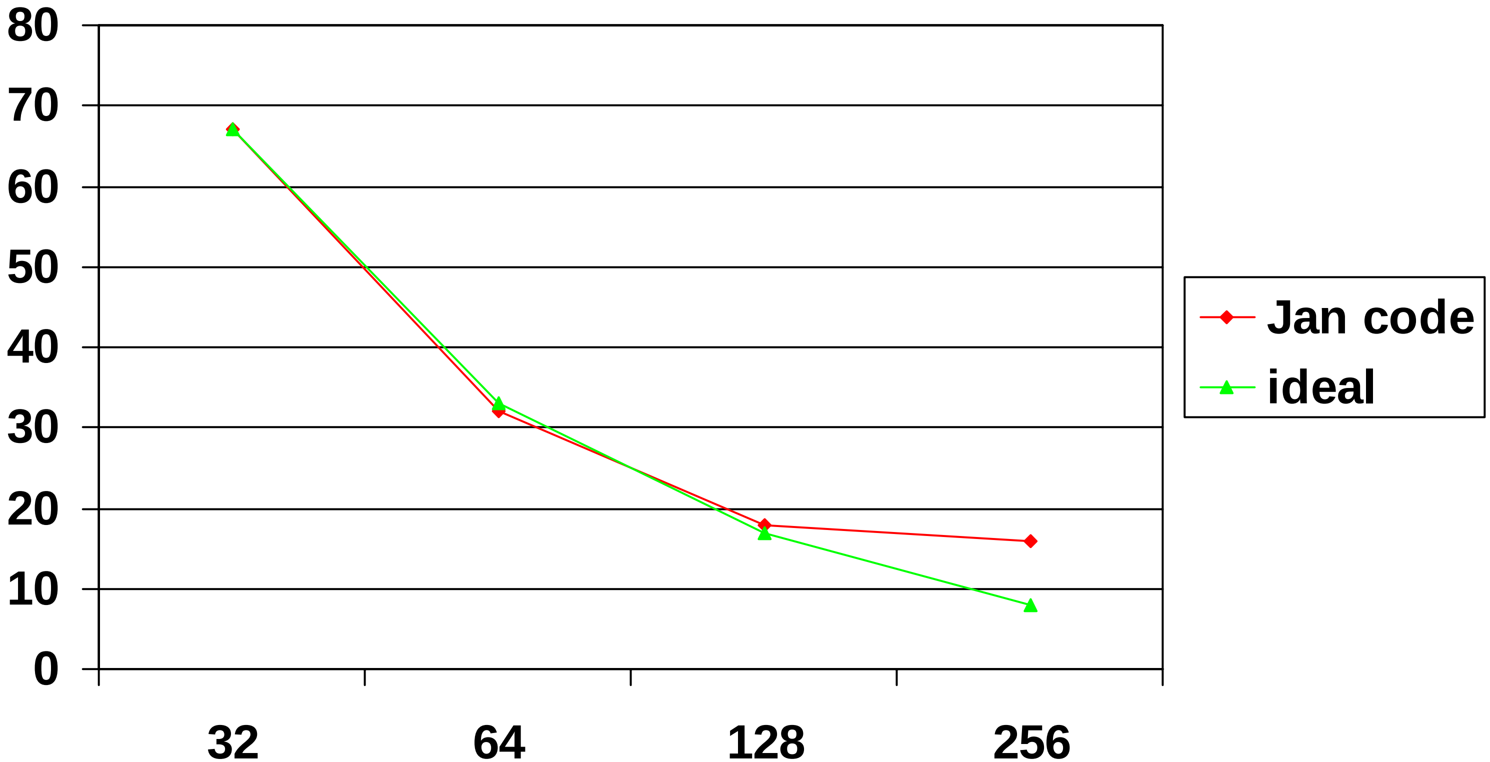
Ar_N Cluster Benchmarks(Performance)

- <u>Specifications</u>
- N=6
- UHF
- C_1 symmetry
- Basis = aug-cc-pvtz (300bf)
- N^{corr}_{occ} = 54
- R = 5 bohr

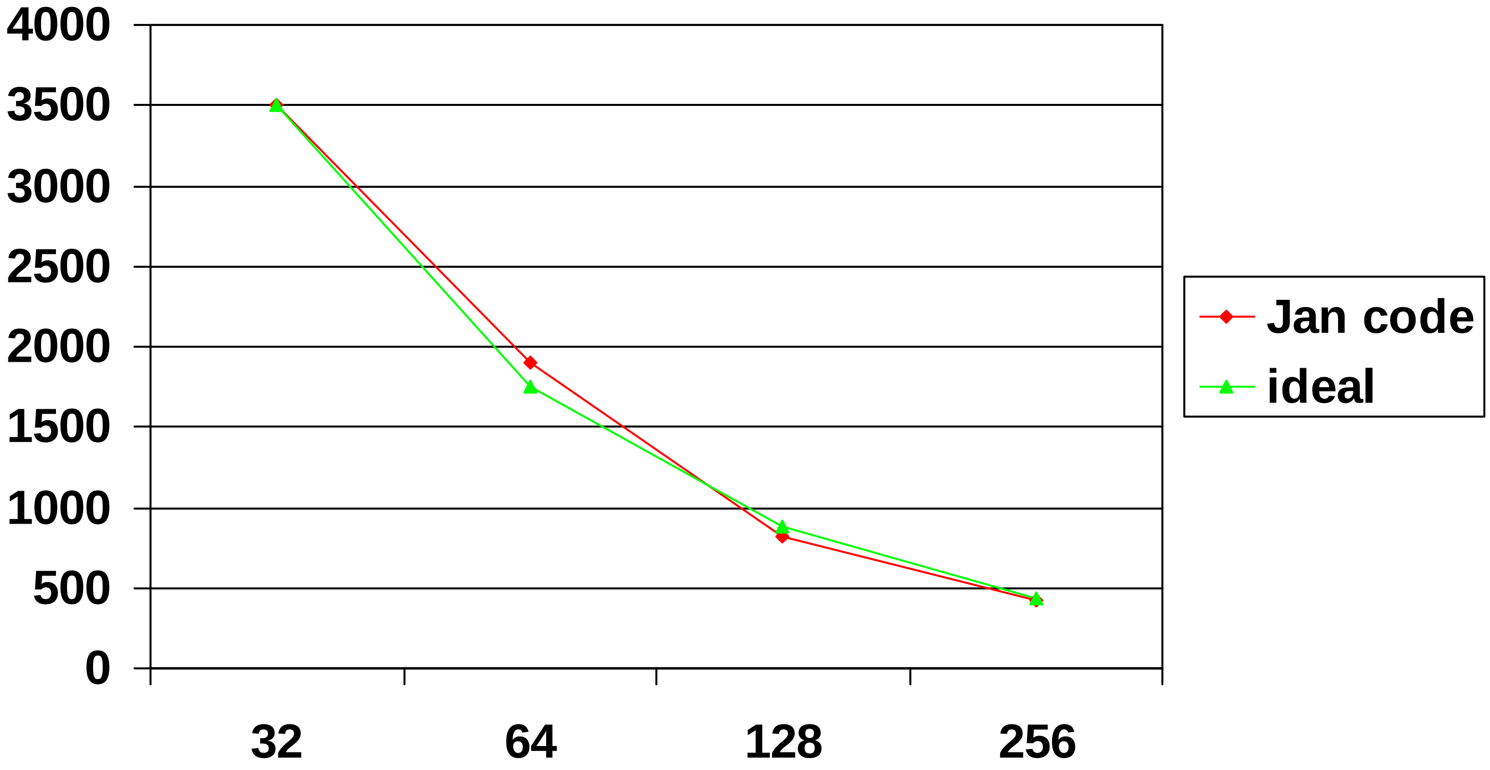
- <u>Methods</u>
- MBPT(2) gradient
- CCSD gradient
- CCSD(T) (core dropped)
- MBPT(2) Hessian (RHF)



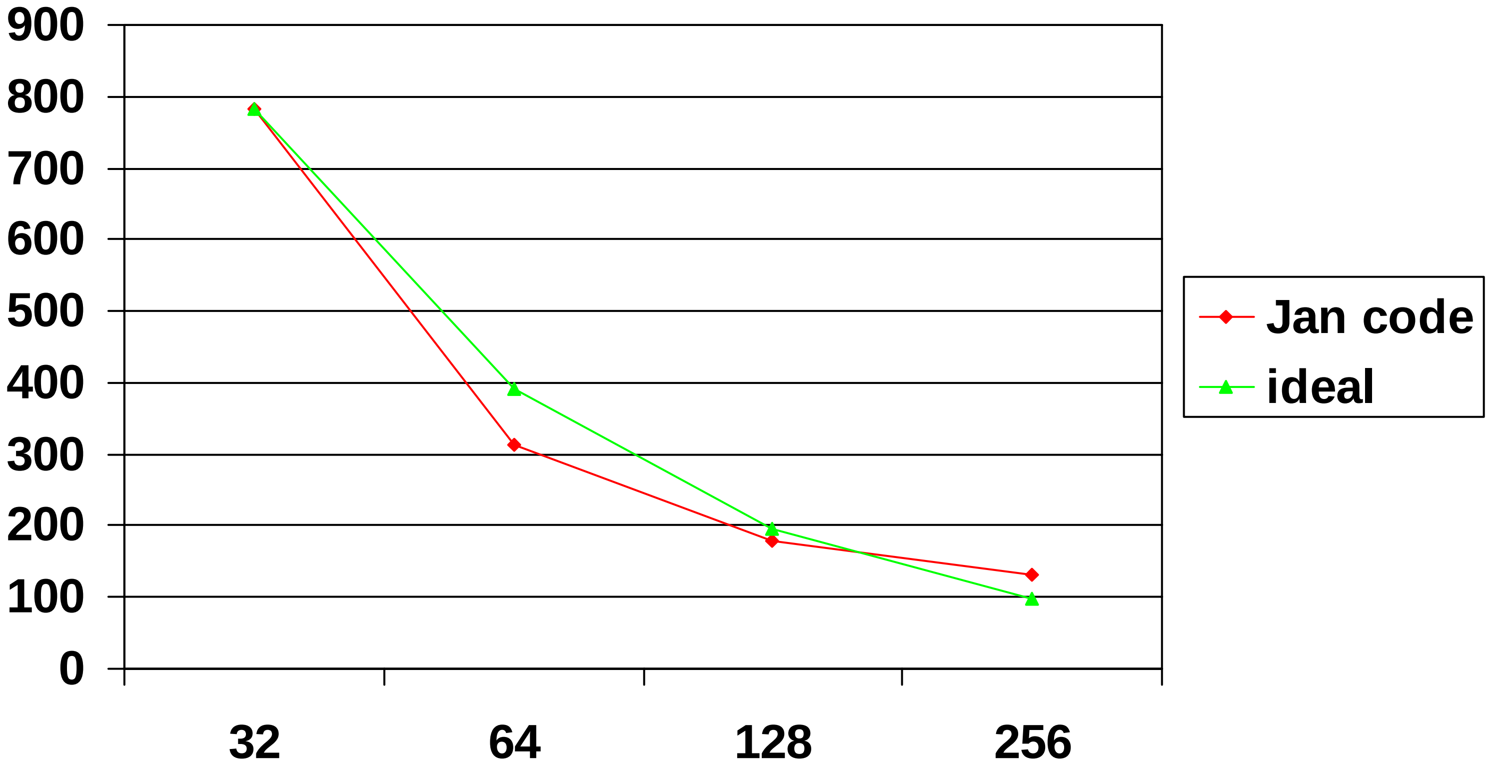
Ar_6 UHF MBPT(2) gradient scaling min per iteration; 54 corr occ alpha



Ar_6 UHF CCSD gradient scaling min per iteration; 54 corr occ alpha



Ar_6 UHF CCSD(T) scaling
min per iteration; 24 corr occ alpha



Ar_6 MBPT(2) Hessian Results

- Asymmetric evaluation algorithm
- $V^* d^2V/dpdq$
- dV/dp
- $d\mathcal{V}/dq$
- $dV/dp^* d\mathcal{V}/dq$
- Number of Hessian elements = 324/2

- Number of processors = 128
- T=381 minutes
- 155 sec / pert p
- 330 sec / pert q
- 16 sec / element

Benchmarks website

- From workshop on “Parallelization of Coupled Cluster Methods”
  - Feb 23-24, 2008 St. Simons Island, Georgia at 2008 Sanibel Symposium
- http://www.qtp.ufl.edu/PCCworkshop/PCCbenchmarks.html

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A single CPU computer

- Basic data item: 64 bit number
- High level language: Fortran, C
  - c = a + b
- Assembly language
  - ADD dest,src
  - ADD is an operation code
  - dest and src are registers

The ACES III machine

- Basic data item: data block 10,000 64 bit numbers -> super number
- High level language: being developed
- Assembly language: SIAL super instruction assembly language
  - R(I,J,K,L) += V(I,J,C,D) * T(C,D,K,L)
- xaces3 -> super instruction processor

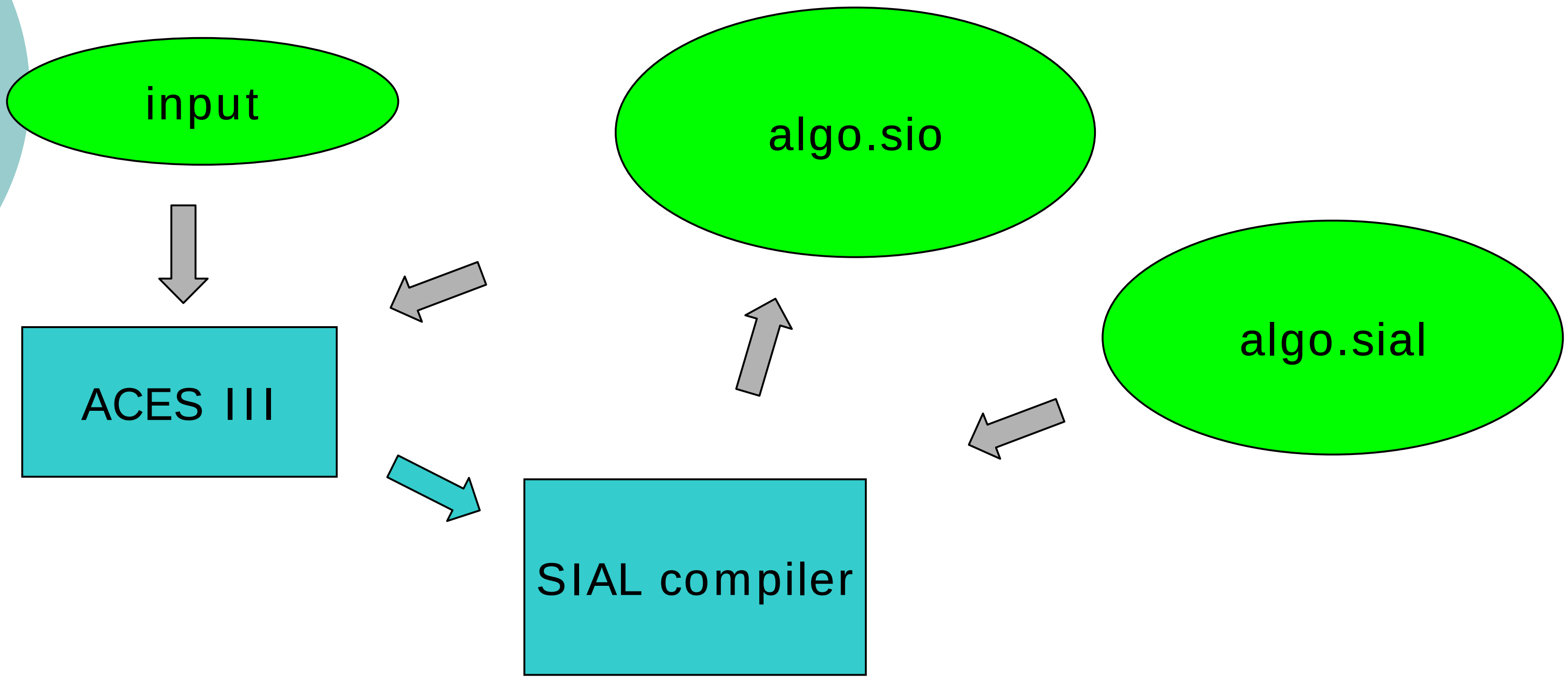
Coarse grain parallelism

- Memory super instruction
  - GET block
- can be from
  - Local node RAM
  - Other node RAM
- Only difference is execution time!

Fine grain parallelism

- Compute super instruction
  - * (contractions)
  - compute_integrals
- can use multiple cores and accelerators like GPU

Execution flow



Distributed data flow

- N worker tasks each with local RAM
- Data distributed in RAM of workers
  - AO-based: direct use of integrals
  - MO-based: use transformed integrals
- Array blocks are spread over all workers
- Workers compute integrals when integral instruction is called

Disk resident data flow

- M server tasks
  - have access to local or global disk storage
  - accept, store and retrieve blocks
  - also compute integrals when asked
- Data served to and from disk

New developments

- Develop higher level programming language
- Data staging
  - Huge served array
  - Copy section in distributed array
  - Work efficiently on distributed array
- Similar to BLAS-3 management of cache

ACES III is ready

- Tackle problems larger than ever
- We are now working on getting some benchmark results on 1,000 and 2,000 processors
  - The problem is getting quick access to 1,000 and 2,000 processors to tune for good performance
  - Running ACES III is easy