A Brief History of the COLUMBUS Program System

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History of COLUMBUS

- **PreCOLUMBUS Software**
  - **I43210 Integrals Program** (1973, Russ Pitzer, Segmented gaussians, symmetry orbital integrals with nonabelian point groups)
  - **UEIL and UCI** (1979, Ron Shepard, Loop-driven GUGA MCSCF and Direct-CI)

- **COLUMBUS (1980-1981)**
  - **I94720** (restricted to D2h and with different file format)
  - **UEXP** (GUGA, Inverted FT based on loop templates with recursion)
  - **CI** (GUGA, MR-SDCI with internal/external orbitals, Inverted FT based on loop templates with recursion)
  - **Integral Transformation (symmetry blocked)**
History of COLUMBUS

(1981-1985)
• Separate Versions Everywhere (OSU, ANL, Vienna, Karlsruhe, Utah, Japan)
• ARGOS (1983, Generally Contracted Basis Functions)
• Matrix-Product Formulation of MR-SDCI (1983)
• Improved CI Diagonalization Algorithms (less I/O, more roots)
• Improved Shavitt-loop generation (stack/tree-search based)
• MCSCF (separate treatment of D/A/V orbitals)
• Incorporated CMDC to help portability (IBM MVS, VAX VMS, Cray CTSS, CDC, Harris, DEC-10/20, Cray COS, Cyber-205, FPS)

(1985-1987)
• Reconciliation of branches (OSU, ANL, Vienna, Karlsruhe)
• Distribution with anonymous FTP (first large quantum chemistry code to do this)
History of COLUMBUS

(1988-1993)

• Coordinated (manual) development effort
• Several production versions were distributed with anonymous FTP
• Old CITRAN replaced by TRAN and CISRT
• SIFS library
• CIDEN and CIGRAD developed (first efficient analytic gradient procedure for MRCI methods, but limited to segmented basis sets and to d-orbitals)
• First ports to unix computers (sun, ardent, stardent, alliant, Cray unicosa, SGI, Fujitsu)
• MR-PT methods added
• Separate development forks for GUGA-Spin-Orbit CI, Trigonometric Interpolation MCSCF, Parallel-CI, AO-Integral based Direct-SCF and CI, SPAM
History of COLUMBUS

(1994-1998)
• Incorporate DALTON for generally-contracted gradient integrals
• First versions of shell scripts to automate the job steps
• First automatic geometry optimization

(1999-present)
• perl scripts control the job steps
• Input simplified for “standard” cases with colinp
• Parallel technology matures (MPI, GA_LIB, linux clusters)
• Parallel CIDEN allows for analytic gradients for large wfns
• Merging of several development forks (Parallel-CI, Spin-Orbit-CI)
• New development projects (nonadiabatic coupling, COSMO)
• Several development forks were terminated (MR-PT, Trigonometric Interpolation MCSCF, AO-integral based CI, SPAM, data compression, TQ excitations) because coarse-grained coordinated development effort is too difficult
• Drop almost all operating system support except unix
• The code is now fragile, it is sometimes difficult to complete a successful installation
History of COLUMBUS

(present-future)

- Use CVS for coordinated distributed development
- More frequent source-code merges allows finer-grained changes
- Use F90/F95/F2003 features to advantage
- Allow code to regain its robustness
- Effort is distributed, not serialized onto a single “librarian”
- Allow research projects to be restarted (MR-PT, SPAM, Data compression, Trigonometric Interpolation, Spin-Orbit-CI Gradients)

One purpose for this workshop is to determine the best way to proceed to achieve these goals