A High-Level Approach to the Synthesis of High-Performance Codes for Quantum Chemistry

Oak Ridge National Laboratory

David E. Bernholdt, Venkatesh Choppella, David Dean, Robert Harrison, Thomas Papenbrock, Michael Strayer, Trey White

Pacific Northwest National Laboratory

So Hirata

Ohio State University

Gerald Baumgartner, Daniel Cociorva, Russ Pitzer, P Sadayappan, a small army of graduate students

Louisiana State University

J Ramanujam

Princeton University

Marcel Nooijen, Alexander Auer

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Problem Domain: High-Accuracy Quantum Chemical Methods

- Coupled cluster methods are widely used for very high quality electronic structure calcs.
- Typical Laplace factorized CCSD(T) term:

Typical methods will have tens to hundreds of such terms

$$A3A = \tfrac{1}{2}\left(X_{ce,af}Y_{ae,cf} + X_{c\bar{e},a\bar{f}}Y_{a\bar{e},c\bar{f}} + X_{\bar{c}\bar{e},af}Y_{\bar{a}\bar{e},cf} + X_{\bar{c}e,a\bar{f}}Y_{ae,\bar{c}\bar{f}} + X_{\bar{c}e,\bar{a}f}Y_{\bar{a}e,\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}}Y_{\bar{a}\bar{e},\bar{c}\bar{f}}\right)$$

$$X_{ce,af} = t_{ij}^{ce}t_{ij}^{af} \qquad Y_{ae,cf} = \langle ab\|ek\rangle\langle cb\|fk\rangle$$

- Indices i, j, k *O*(O=100) values, a, b, c, e, f *O*(V=3000)
- Term costs *O*(OV^5) $\approx 10^{19}$ FLOPs; Integrals ~ 1000 FLOPs each
- *O*(V^4) terms ~ 500 TB memory each

The “Tensor Contraction Engine” (TCE) Concept

- User describes computational problem (tensor contractions, a la many-body methods) in a simple, high-level language
  - Similar to what might be written in papers
- Compiler-like tools translate high-level language into traditional Fortran (or C, or…) code
- Generated code is compiled and linked to libraries providing computational infrastructure

Addressing Programming Challenges

- **Productivity**
  - User writes simple, high-level code
  - Code generation tools do the tedious work
- **Complexity**
  - Significantly reduces complexity visible to programmer
- **Performance**
  - Perform optimizations prior to code generation
  - Automate many decisions humans make empirically
  - Tailor generated code to target computer
  - Tailor generated code to specific problem

So What's New About This Project?

- The creation of "little languages" and code generation tools has a long history in chemistry and other domains
- **Usually viewed only as productivity tools**
  - Imitate what researcher would do – but quicker
- **We treat it as a computer science problem**
  - Similar to (not identical to) an optimizing compiler
  - Algorithmic choices are explored and evaluated rigorously and (in most cases) exhaustively
  - Make use of machine architecture & performance models to specialize generated code to target system
- **Target applications**
  - Rapid experimentation with new many-body methods
  - Implementation of high-complexity methods
  - Improving computational efficiency on parallel machines
  - Also for nuclear physics…

A High-Level Language for Tensor Contraction Expressions

$$A3A = \tfrac{1}{2}\left(X_{ce,af} Y_{ae,cf} + X_{c\bar{e},a\bar{f}} Y_{a\bar{e},c\bar{f}} + X_{\bar{c}\bar{e},af} Y_{\bar{a}\bar{e},cf} + X_{\bar{c}e,a\bar{f}} Y_{ae,\bar{c}\bar{f}} + X_{\bar{c}e,\bar{a}f} Y_{\bar{a}e,\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}} Y_{\bar{a}\bar{e},\bar{c}\bar{f}} \right)$$

$$X_{ce,af} = t_{ij}^{ce} t_{ij}^{af} \qquad Y_{ae,cf} = \langle ab \| ek \rangle \langle cb \| fk \rangle$$

```
range V = 3000;
range O = 100;

index a,b,c,d,e,f : V;
index i,j,k : O;

mlimit = 10000000000000;

function F1(V,V,V,O);
function F2(V,V,V,O);

procedure P(in T1[O,O,V,V], in T2[O,O,V,V], out X)=

begin
   X == sum[ sum[F1(a,b,f,k) * F2(c,e,b,k), {b,k}]
                 * sum[T1[i,j,a,e] * T2[i,j,c,f], {i,j}],
                 {a,e,c,f}];
end
```

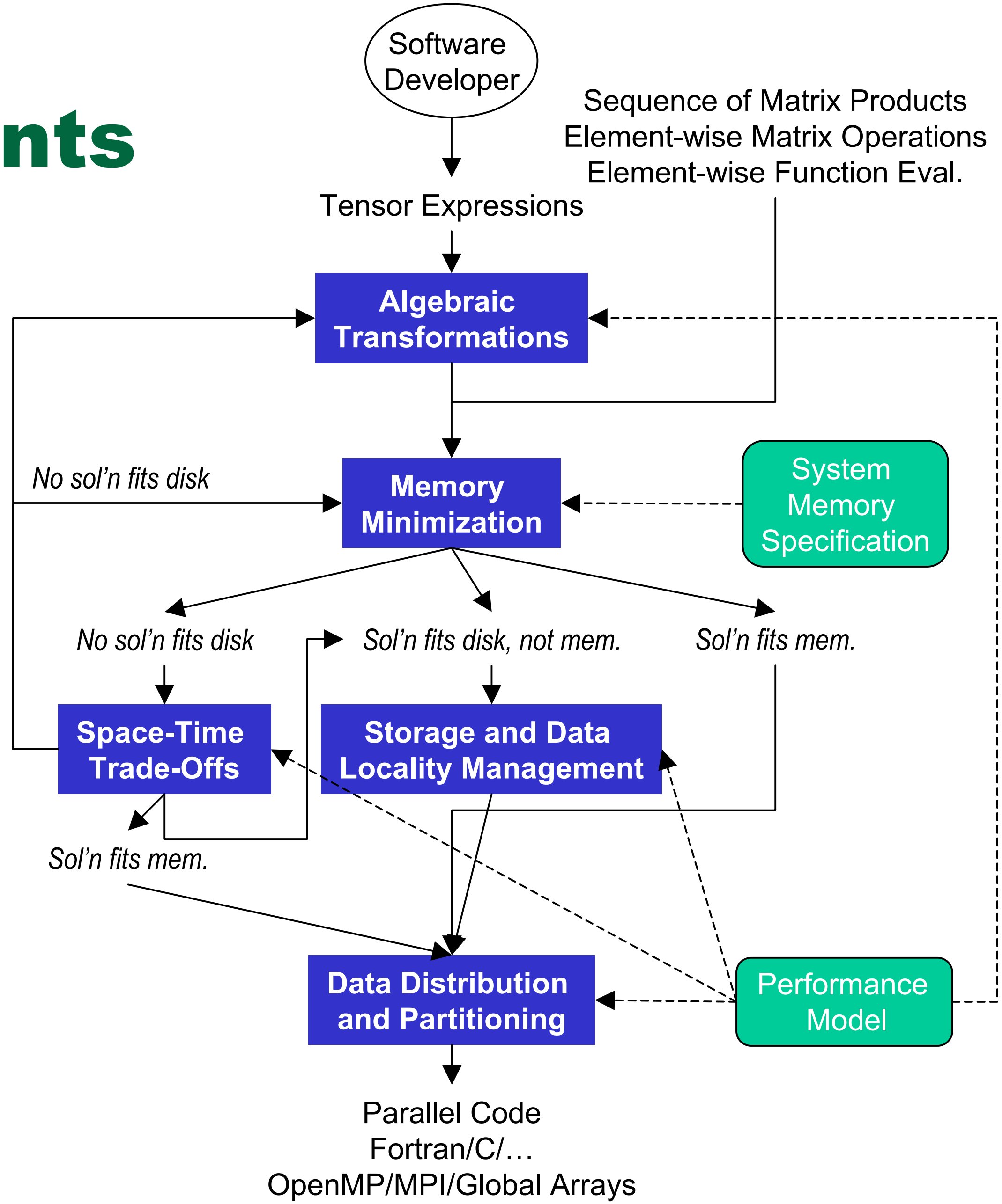
CCSD Doubles Equation

```
hbar[a,b,i,j] == sum[f[b,c]*t[i,j,a,c],{c}] -sum[f[k,c]*t[k,b]*t[i,j,a,c],{k,c}] +sum[f[a,c]*t[i,j,c,b],{c}] -sum[f[k,c]*t[k,a]*t[i,j,c,b],{k,c}] -
    sum[f[k,j]*t[i,k,a,b],{k}] -sum[f[k,c]*t[j,c]*t[i,k,a,b],{k,c}] -sum[f[k,i]*t[j,k,b,a],{k}] -sum[f[k,c]*t[i,c]*t[j,k,b,a],{k,c}]
    +sum[t[i,c]*t[j,d]*v[a,b,c,d],{c,d}] +sum[t[i,j,c,d]*v[a,b,c,d],{c,d}] +sum[t[j,c]*v[a,b,i,c],{c}] -sum[t[k,b]*v[a,k,i,j],{k}]
    +sum[t[i,c]*v[b,a,j,c],{c}] -sum[t[k,a]*v[b,k,j,i],{k}] -sum[t[k,d]*t[i,j,c,b]*v[k,a,c,d],{k,c,d}] -sum[t[i,c]*t[j,k,b,d]*v[k,a,c,d],{k,c,d}] -
    sum[t[j,c]*t[k,b]*v[k,a,c,i],{k,c}] +2*sum[t[j,k,b,c]*v[k,a,c,i],{k,c}] -sum[t[j,k,c,b]*v[k,a,c,i],{k,c}] -sum[t[i,c]*t[j,d]*t[k,b]*v[k,a,d,c],{k,c,d}]
    +2*sum[t[k,d]*t[i,j,c,b]*v[k,a,d,c],{k,c,d}] -sum[t[k,b]*t[i,j,c,d]*v[k,a,d,c],{k,c,d}] -sum[t[j,d]*t[i,k,c,b]*v[k,a,d,c],{k,c,d}]
    +2*sum[t[i,c]*t[j,k,b,d]*v[k,a,d,c],{k,c,d}] -sum[t[i,c]*t[j,k,d,b]*v[k,a,d,c],{k,c,d}] -sum[t[j,k,b,c]*v[k,a,i,c],{k,c}] -
    sum[t[i,c]*t[k,b]*v[k,a,j,c],{k,c}] -sum[t[i,k,c,b]*v[k,a,j,c],{k,c}] -sum[t[i,c]*t[j,d]*t[k,a]*v[k,b,c,d],{k,c,d}] -
    sum[t[k,d]*t[i,j,a,c]*v[k,b,c,d],{k,c,d}] -sum[t[k,a]*t[i,j,c,d]*v[k,b,c,d],{k,c,d}] +2*sum[t[j,d]*t[i,k,a,c]*v[k,b,c,d],{k,c,d}] -
    sum[t[j,d]*t[i,k,c,a]*v[k,b,c,d],{k,c,d}] -sum[t[i,c]*t[j,k,d,a]*v[k,b,c,d],{k,c,d}] -sum[t[i,c]*t[k,a]*v[k,b,c,j],{k,c}]
    +2*sum[t[i,k,a,c]*v[k,b,c,j],{k,c}] -sum[t[i,k,c,a]*v[k,b,c,j],{k,c}] +2*sum[t[k,d]*t[i,j,a,c]*v[k,b,d,c],{k,c,d}] -
    sum[t[j,d]*t[i,k,a,c]*v[k,b,d,c],{k,c,d}] -sum[t[j,c]*t[k,a]*v[k,b,i,c],{k,c}] -sum[t[j,k,c,a]*v[k,b,i,c],{k,c}] -sum[t[i,k,a,c]*v[k,b,j,c],{k,c}]
    +sum[t[i,c]*t[j,d]*t[k,a]*t[l,b]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[k,b]*t[l,d]*t[i,j,a,c]*v[k,l,c,d],{k,l,c,d}] -
    2*sum[t[k,a]*t[l,d]*t[i,j,c,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[k,a]*t[l,b]*t[i,j,c,d]*v[k,l,c,d],{k,l,c,d}] -
    2*sum[t[j,c]*t[l,d]*t[i,k,a,b]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[j,d]*t[l,b]*t[i,k,a,c]*v[k,l,c,d],{k,l,c,d}]
    +sum[t[j,d]*t[l,b]*t[i,k,c,a]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,c]*t[l,d]*t[j,k,b,a]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,a]*t[j,k,b,d]*v[k,l,c,d],{k,l,c,d}]
    +sum[t[i,c]*t[l,b]*t[j,k,d,a]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,k,c,d]*t[j,l,b,a]*v[k,l,c,d],{k,l,c,d}] +4*sum[t[i,k,a,c]*t[j,l,b,d]*v[k,l,c,d],{k,l,c,d}] -
    2*sum[t[i,k,c,a]*t[j,l,b,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,k,a,b]*t[j,l,c,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,k,a,c]*t[j,l,d,b]*v[k,l,c,d],{k,l,c,d}]
    +sum[t[i,k,c,a]*t[j,l,d,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,c]*t[j,d]*t[k,l,a,b]*v[k,l,c,d],{k,l,c,d}] +sum[t[i,j,c,d]*t[k,l,a,b]*v[k,l,c,d],{k,l,c,d}] -
    2*sum[t[i,j,c,b]*t[k,l,a,d]*v[k,l,c,d],{k,l,c,d}] -2*sum[t[i,j,a,c]*t[k,l,b,d]*v[k,l,c,d],{k,l,c,d}] +sum[t[j,c]*t[k,b]*t[l,a]*v[k,l,c,i],{k,l,c}]
    +sum[t[l,c]*t[j,k,b,a]*v[k,l,c,i],{k,l,c}] -2*sum[t[l,a]*t[j,k,b,c]*v[k,l,c,i],{k,l,c}] +sum[t[l,a]*t[j,k,c,b]*v[k,l,c,i],{k,l,c}] -
    2*sum[t[k,c]*t[j,l,b,a]*v[k,l,c,i],{k,l,c}] +sum[t[k,a]*t[j,l,b,c]*v[k,l,c,i],{k,l,c}] +sum[t[k,b]*t[j,l,c,a]*v[k,l,c,i],{k,l,c}]
    +sum[t[j,c]*t[l,k,a,b]*v[k,l,c,i],{k,l,c}] +sum[t[i,c]*t[k,a]*t[l,b]*v[k,l,c,j],{k,l,c}] +sum[t[l,c]*t[i,k,a,b]*v[k,l,c,j],{k,l,c}] -
    2*sum[t[l,b]*t[i,k,a,c]*v[k,l,c,j],{k,l,c}] +sum[t[l,b]*t[i,k,c,a]*v[k,l,c,j],{k,l,c}] +sum[t[i,c]*t[k,l,a,b]*v[k,l,c,j],{k,l,c}]
    +sum[t[j,c]*t[l,d]*t[i,k,a,b]*v[k,l,d,c],{k,l,c,d}] +sum[t[j,d]*t[l,b]*t[i,k,a,c]*v[k,l,d,c],{k,l,c,d}] +sum[t[j,d]*t[l,a]*t[i,k,c,b]*v[k,l,d,c],{k,l,c,d}] -
    2*sum[t[i,k,c,d]*t[j,l,b,a]*v[k,l,d,c],{k,l,c,d}] -2*sum[t[i,k,a,c]*t[j,l,b,d]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,c,a]*t[j,l,b,d]*v[k,l,d,c],{k,l,c,d}]
    +sum[t[i,k,a,b]*t[j,l,c,d]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,c,b]*t[j,l,d,a]*v[k,l,d,c],{k,l,c,d}] +sum[t[i,k,a,c]*t[j,l,d,b]*v[k,l,d,c],{k,l,c,d}]
    +sum[t[k,a]*t[l,b]*v[k,l,i,j],{k,l}] +sum[t[k,l,a,b]*v[k,l,i,j],{k,l}] +sum[t[k,b]*t[l,d]*t[i,j,a,c]*v[l,k,c,d],{k,l,c,d}]
    +sum[t[k,a]*t[l,d]*t[i,j,c,b]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,c]*t[l,d]*t[j,k,b,a]*v[l,k,c,d],{k,l,c,d}] -2*sum[t[i,c]*t[l,a]*t[j,k,b,d]*v[l,k,c,d],{k,l,c,d}]
    +sum[t[i,c]*t[l,a]*t[j,k,d,b]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,j,c,b]*t[k,l,a,d]*v[l,k,c,d],{k,l,c,d}] +sum[t[i,j,a,c]*t[k,l,b,d]*v[l,k,c,d],{k,l,c,d}] -
    2*sum[t[l,c]*t[i,k,a,b]*v[l,k,c,j],{k,l,c}] +sum[t[l,b]*t[i,k,a,c]*v[l,k,c,j],{k,l,c}] +sum[t[l,a]*t[i,k,c,b]*v[l,k,c,j],{k,l,c}] +v[a,b,i,j]
```

In the coupled cluster method with single and double excitations (CCSD) the “singles” and “doubles” equations are iterated until convergence and that solution is used to evaluate the molecular energy

TCE Components

- Algebraic Transformations
  - Minimize operation count
- Memory Minimization
  - Reduce intermediate storage
- Space-Time Transformation
  - Trade-offs btw storage and recomputation
- Storage Management and Data Locality Optimization
  - Optimize use of storage hierarchy
- Data Distribution and Partitioning
  - Optimize parallel layout



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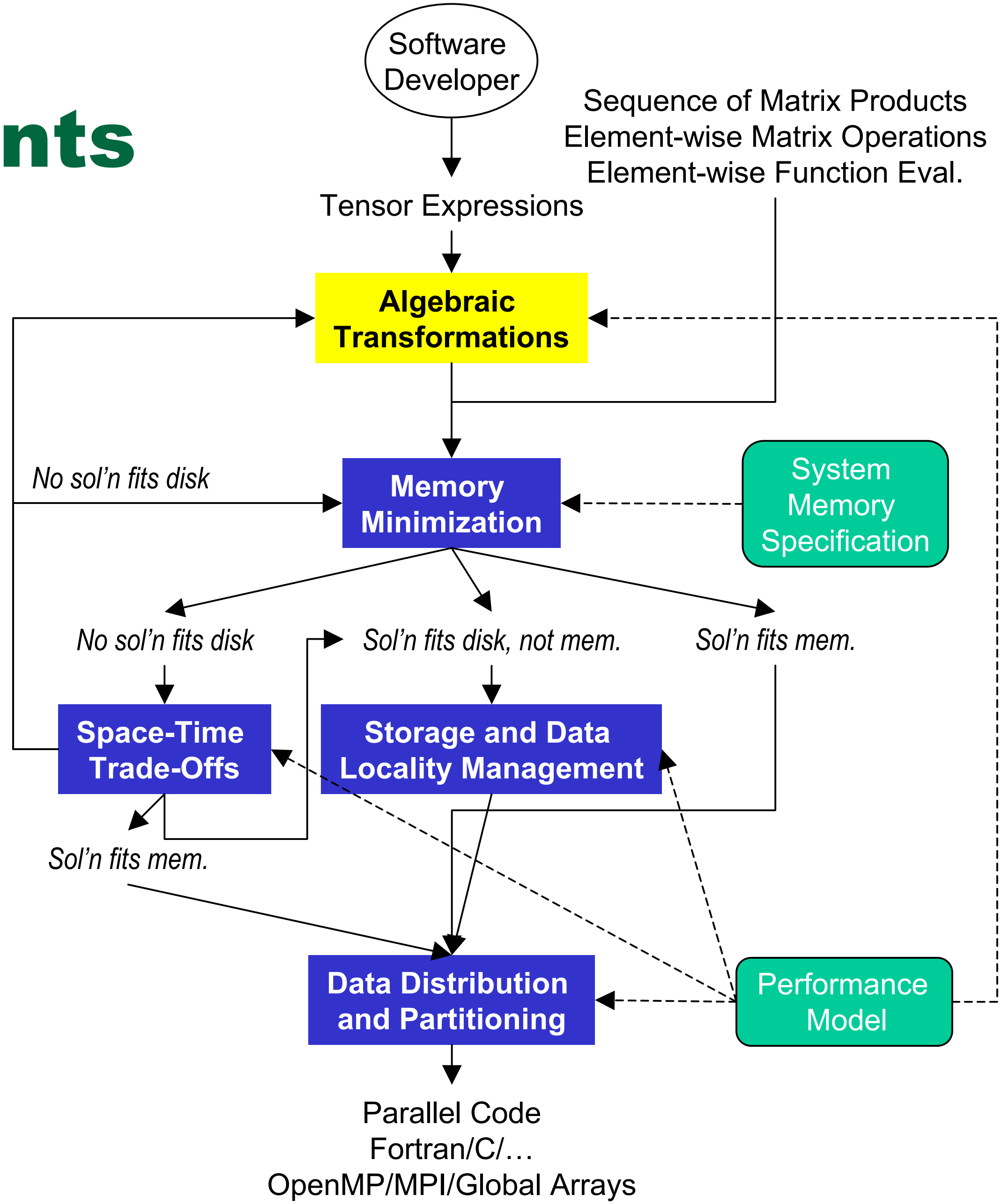

Algebraic Transformations: Operation Minimization

$$S(a,b,i,j) = \sum_{c,d,e,f,k,l} A(a,c,i,k)B(b,e,f,l)C(d,f,j,k)D(c,d,e,l)$$

- Requires $4 * N^{10}$ operations if indices a-l have range N

- Using associative, commutative, distributive laws acceptable
- Optimal formula sequence requires only $6 * N^6$ operations

$$T1(b,c,d,f) = \sum_{e,l} B(b,e,f,l)D(c,d,e,l)$$

$$T2(b,c,j,k) = \sum_{d,f} T1(b,c,d,f)C(d,f,j,k)$$

$$S(a,b,i,j) = \sum_{c,k} T2(b,c,j,k)A(a,c,i,k)$$

Memory Minimization: Loop Fusion

Formula sequence

$$T1_{bcdf} = \sum_{e,l} B_{befl} D_{cdel}$$

$$T2_{bcjk} = \sum_{d,f} T1_{bcdf} C_{dfjk}$$

$$S_{abij} = \sum_{c,k} T2_{bcjk} A_{acik}$$

Unfused code

```
T1 = 0; T2 = 0; S = 0
for b, c, d, e, f, l
    T1bcdf += Bbefl Dcdel
for b, c, d, f, j, k
    T2bcjk += T1bcdf Cdfjk
for a, b, c, i, j, k
    Sabij += T2bcjk Aacik
```

Fused code

```
S = 0
for b, c
    T1f = 0; T2f = 0
    for d, f
        for e, l
            T1f += Bbefl Dcdel
        for j, k
            T2fjk += T1f Cdfjk
    for a, i, j, k
        Sabij += T2fjk Aacik
```

Operation Minimal Form

```
for a, e, c, f
  for i, j
    X_aecf += T_ijae T_ijcf
for c, e, b, k
  T1_cebk = f1(c, e, b, k)
for a, f, b, k
  T2_afbk = f2(a, f, b, k)
for c, e, a, f
  for b, k
    Y_ceaf += T1_cebk T2_afbk
for c, e, a, f
  E += X_aecf Y_ceaf
```

Inputs: T_{ijae}, T_{ijcf}

External function calls: f1, f2

Output: E

array	space	time
X	V^4	V^4O^2
T1	V^3O	$C_{f1}V^3O$
T2	V^3O	$C_{f2}V^3O$
Y	V^4	V^5O
E	1	V^4

a .. f: range V = 1000 .. 3000

i .. k: range O = 30 .. 100

$$A3A = \tfrac{1}{2}\left(X_{ce,af}Y_{ae,cf} + X_{c\bar{e},a\bar{f}}Y_{a\bar{e},c\bar{f}} + X_{\bar{c}\bar{e},af}Y_{\bar{a}\bar{e},cf} + X_{\bar{c}e,a\bar{f}}Y_{ae,\bar{c}\bar{f}} + X_{\bar{c}e,\bar{a}f}Y_{\bar{a}e,\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}}Y_{\bar{a}\bar{e},\bar{c}\bar{f}}\right)$$

$$X_{ce,af} = t_{ij}^{ce} t_{ij}^{af} \qquad Y_{ae,cf} = \langle ab \| ek \rangle \langle cb \| fk \rangle$$

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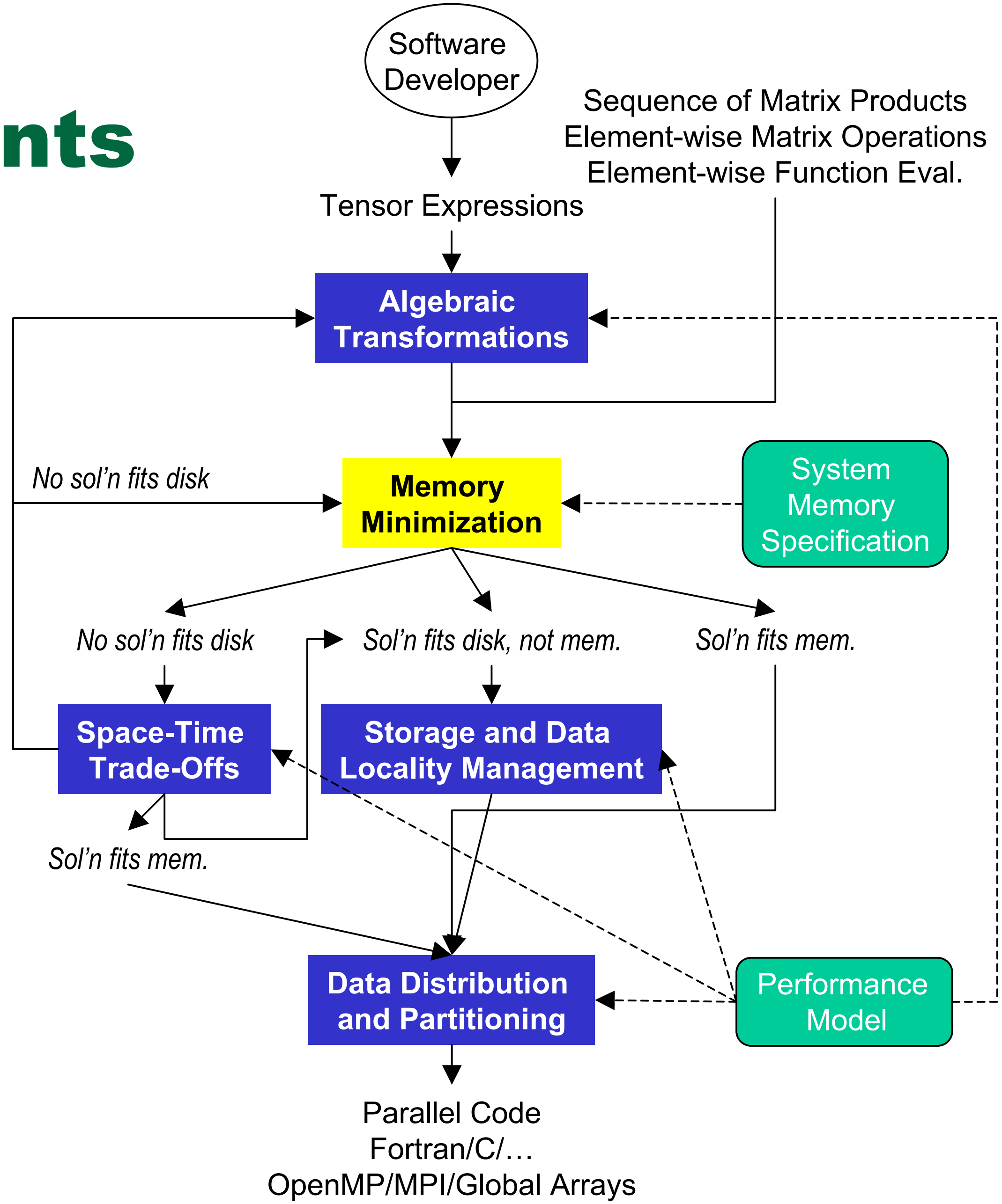

Memory-Minimal Form

Fusion of loops allows reduction of rank of arrays

```
for a, f, b, k
[ T2_afbk = f2(a, f, b, k)
for c, e
[ for b, k
[ [ T1_bk = f1(c, e, b, k)
[ for a, f
[ [ for i, j
[ [ [ X += T_ijae T_ijcf
[ [ for b, k
[ [ [ Y += T1_bk T2_afbk
[ [ E += X Y
```

array	space	time
X	1	V^4O^2
T1	VO	$C_{f1}V^3O$
T2	V^3O	$C_{f2}V^3O$
Y	1	V^5O
E	1	V^4

a .. f: range V = 3000
i .. k: range O = 100

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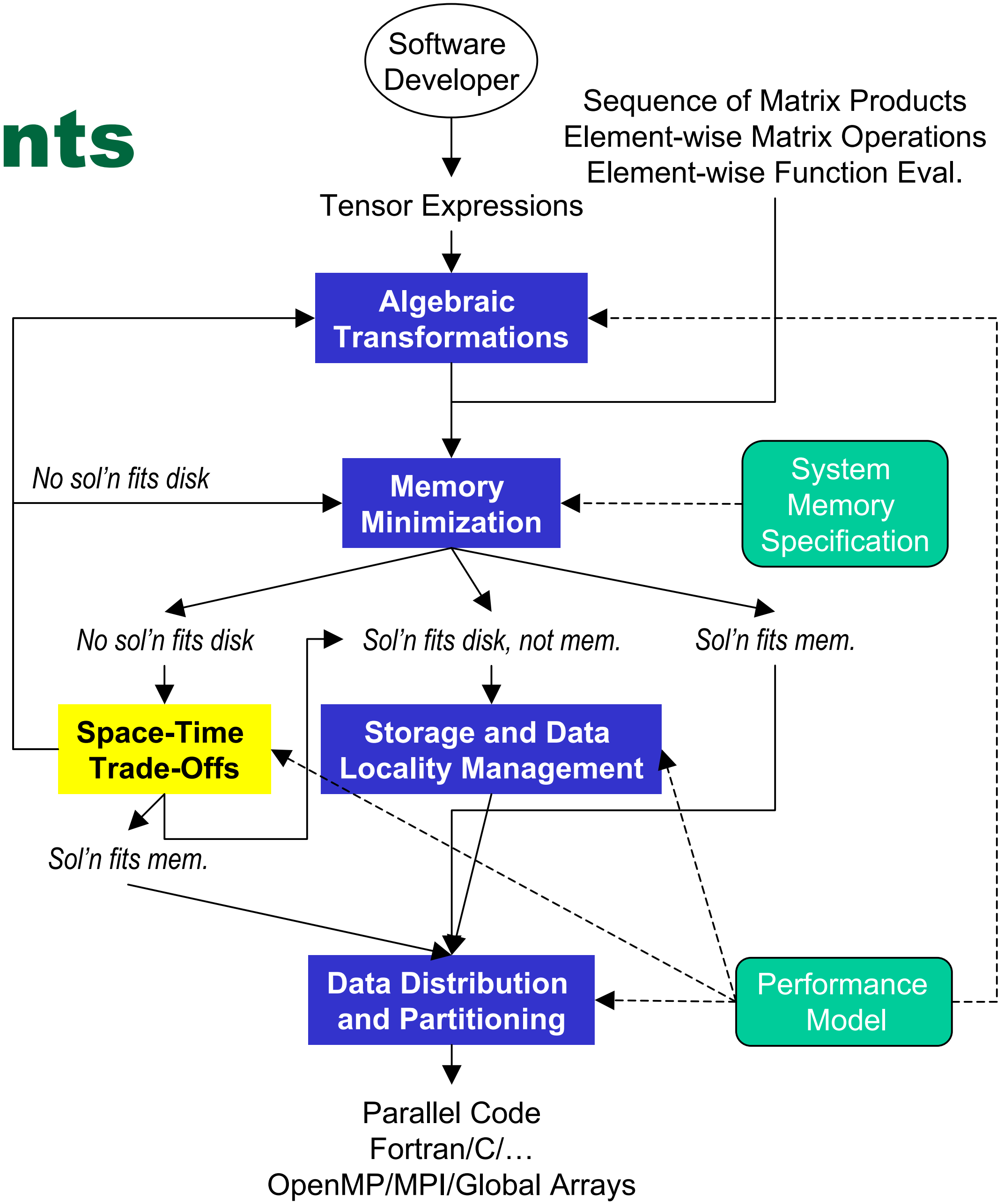

Redundant Computation Allows Full Fusion

```
for a, e, c, f
    for i, j
        X += T_ijae T_ijcf
    for b, k
        T1 = f1(c, e, b, k)
        T2 = f2(a, f, b, k)
        Y += T1 T2
    E += X Y
```

array	space	time
X	1	V^4O^2
T1	1	$C_{f1}V^5O$
T2	1	$C_{f2}V^5O$
Y	1	V^5O
E	1	V^4

Tiling to Reduce Recomputation

for a^t, e^t, c^t, f^t

  for a, e, c, f

    for i, j

      $X_{aecf} \mathrel{+}= T_{ijae} T_{ijcf}$

  for b, k

    for c, e

      $T1_{ce} = f1(c, e, b, k)$

    for a, f

      $T2_{af} = f2(a, f, b, k)$

    for c, e, a, f

      $Y_{ceaf} \mathrel{+}= T1_{ce} T2_{af}$

  for c, e, a, f

    $E \mathrel{+}= X_{aecf} Y_{ceaf}$

array	space	time
X	B^4	V^4O^2
T1	B^2	$C_{f1}(V/B)^2V^3O$
T2	B^2	$C_{f2}(V/B)^2V^3O$
Y	B^4	V^5O
E	1	V^4

![ORNL Oak Ridge National Laboratory]

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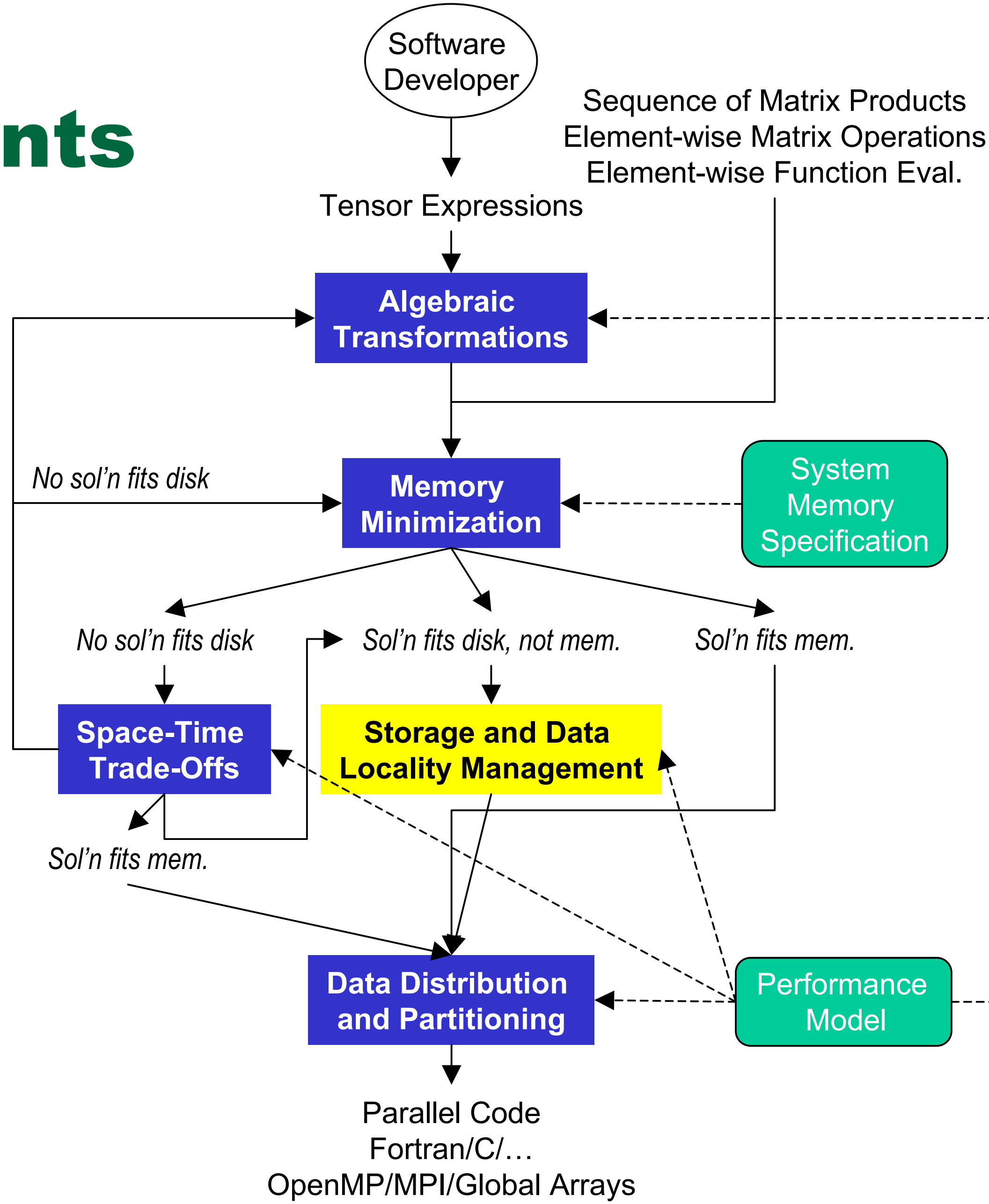
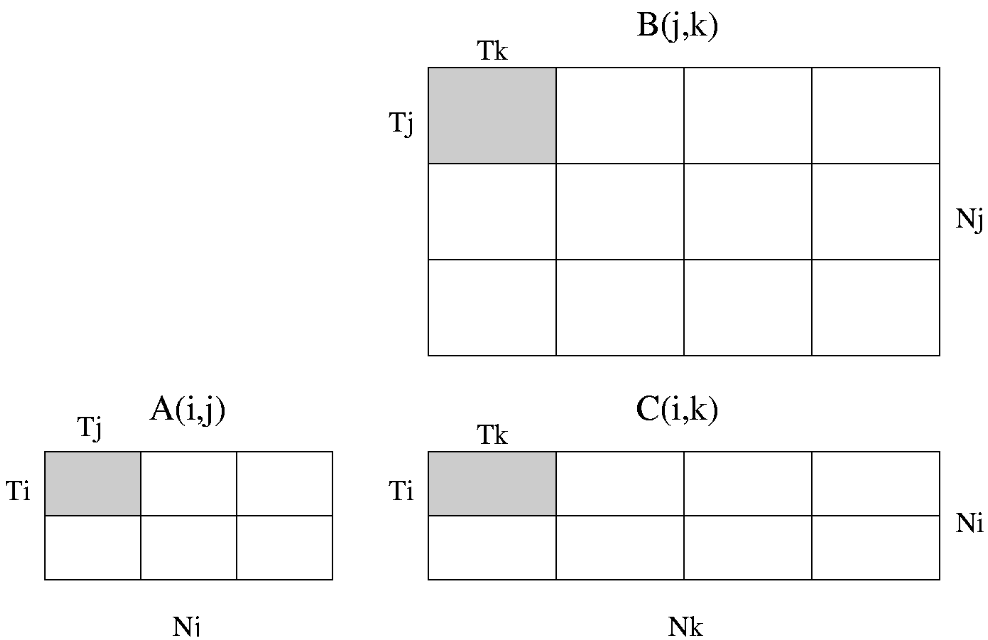


Tiling to Minimize Memory Access Time




```
FOR ii = 1, Ni, Ti
    FOR jj = 1, Nj, Tj
        FOR kk = 1, Nk, Tk
            FOR i = ii, ii + Ti - 1
                FOR j = jj, jj + Tj - 1
                    FOR k = kk, kk + Tk - 1
                        C(i,k) = C(i,k) + A(i,j) * B(j,k)
END FOR k, j, i, kk, jj, ii
```

Choose Ti, Tj, and Tk such that Ti * Tj + Ti * Tk + Tj * Tk < cache size

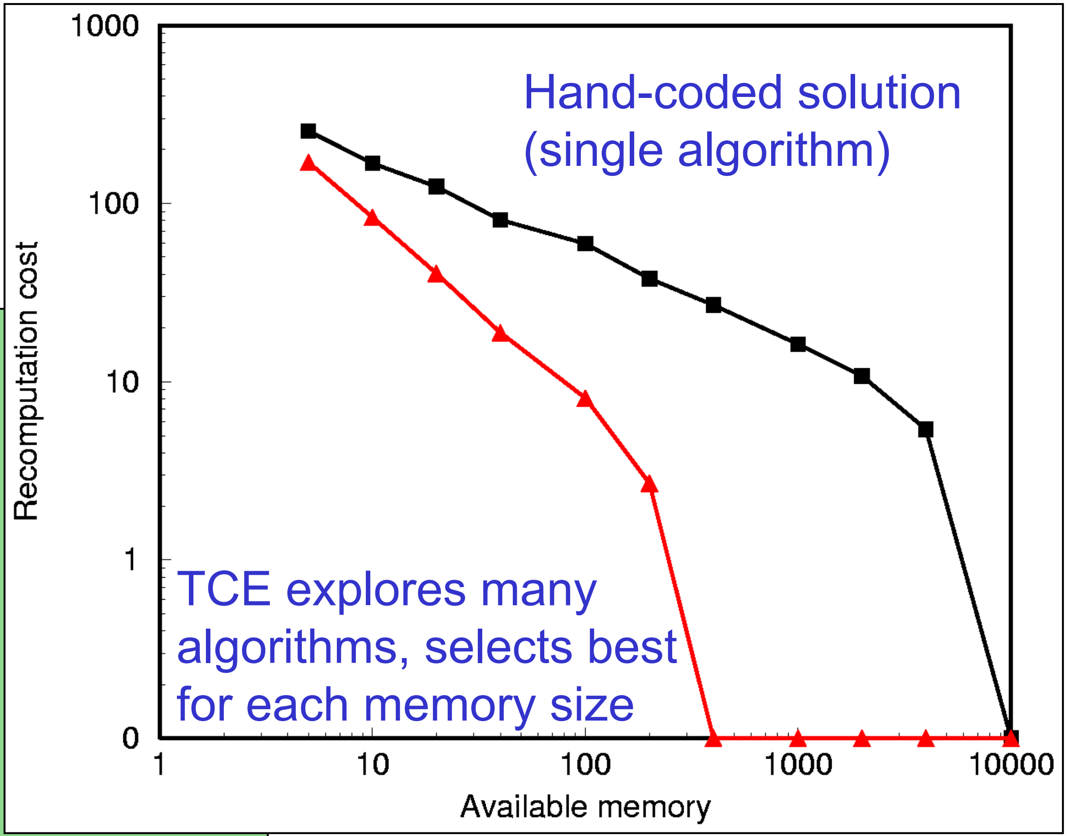
Number of cache misses:

- A(i,j): Ni * Nj
- B(j,k): Nj * Nk * Ni/Ti
- C(i,k): Ni * Nk * Nj/Tj

Same algorithm used to manage locality in disk-based algorithms

The TCE in Operation (Space-Time Trade-Offs)

```
range V = 3000;
range O = 100;

index a,b,c,d,e,f : V;
index i,j,k : O;

mlimit = 1000000000000;

function F1(V,V,V,O);
function F2(V,V,V,O);

procedure P(in T1[O,O,V,V], in T2[O,O,V,V], out X)=

begin
   X == sum[ sum[F1(a,b,f,k) * F2(c,e,b,k), {b,k}]
                 * sum[T1[i,j,a,e] * T2[i,j,c,f], {i,j}],
                 {a,e,c,f}];
end
```



$$A3A = \tfrac{1}{2}\left(X_{ce,af}Y_{ae,cf} + X_{c\bar{e},a\bar{f}}Y_{a\bar{e},c\bar{f}} + X_{\bar{c}\bar{e},af}Y_{\bar{a}\bar{e},cf} + X_{\bar{c}e,a\bar{f}}Y_{ae,\bar{c}\bar{f}} + X_{\bar{c}e,\bar{a}f}Y_{\bar{a}e,\bar{c}f} + X_{\bar{c}\bar{e},\bar{a}\bar{f}}Y_{\bar{a}\bar{e},\bar{c}\bar{f}}\right)$$

$$X_{ce,af} = t_{ij}^{ce} t_{ij}^{af} \qquad Y_{ae,cf} = \langle ab \| ek \rangle \langle cb \| fk \rangle$$

Work in Progress and Planned

- Parallel code generation
  - Data distribution interacts w/ memory minimization and are being combined
  - Multi-level parallelism
- More sophisticated performance models
- Common sub-expression elimination
  - Greatly increases complexity of operation min.
- Chemistry-specific optimizations
  - Automatic use of permutational symmetry
  - Code generation with geometric symmetry
    - May include in cost analysis for extreme calcs.
- Develop approximate algorithms for opt.
  - Address situations where exhaustive search too expensive
  - Deliver best result spending at most 15 min on code gen.
  - Deliver best result spending at most 3 days on code gen.

Summary

- Automatic generation of code from high-level algebraic expressions
  - Approach problem like a compiler
  - Use of HLL allows automation of design decisions usually made by human software developer
- Addresses productivity, complexity, and performance
- Strong interdisciplinary collaboration between chemists and computer scientists
  - Problem from chemists, solutions from computer scientists (w/ significant help from chemists)

For more information

http://www.cis.ohio-state.edu/~gb/TCE

Email: *bernholdtde@ornl.gov*