MADNESS - parallel runtime and application use cases

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Molecular Science Software Project

MS3
MOLECULAR SCIENCE SOFTWARE SUITE

ECCE
EXTENSIBLE COMPUTATIONAL CHEMISTRY ENVIRONMENT

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

GA TOOLS
PARALLEL COMPUTING LIBRARIES AND SOFTWARE TOOLS

<u>PNNL</u>
Yuri Alexeev, Eric Bylaska, Bert deJong, Mahin Hackler, Karol Kowalski, Lisa Pollack, Tjerk Straatsma, Marat Valiev, Edo Apra

<u>ISU and Ames</u>
Theresa Windus

<u>SBU & BNL</u>
Robert Harrison

http://www.nwchem-sw.org

(Jarek Nieplocha), Manoj Krishnan, Bruce Palmer, Daniel Chavarría, Sriram Krishnamoorthy

Gary Black, Brett Didier, Todd Elsenthagen, Sue Havre, Carina Lansing, Bruce Palmer, Karen Schuchardt, Lisong Sun, Erich Vorpagel

Fock matrix in a Nutshell

$$F_{ij} = \sum_{kl} \left(2(ij|kl) - (ik|jl)\right) D_{kl}$$

$$(\mu\nu|\sigma\lambda) = \int_{-\infty}^{\infty} g_\mu(r_1) g_\nu(r_1) \frac{1}{r_{12}} g_\sigma(r_2) g_\lambda(r_2) dr_1 dr_2$$

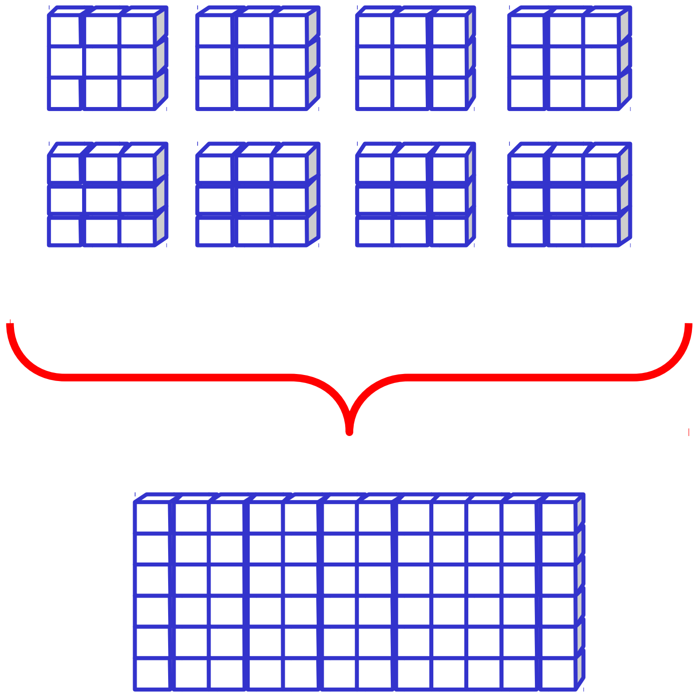
1 integral contributes to 6 Fock Matrix elements

$$(\mu\nu|\sigma\lambda) \otimes \begin{Bmatrix} D_{\mu\nu} \\ D_{\mu\sigma} \\ D_{\mu\lambda} \\ D_{\nu\sigma} \\ D_{\nu\lambda} \\ D_{\sigma\lambda} \end{Bmatrix} \Rightarrow \begin{Bmatrix} F_{\mu\nu} \\ F_{\mu\sigma} \\ F_{\mu\lambda} \\ F_{\nu\sigma} \\ F_{\nu\lambda} \\ F_{\sigma\lambda} \end{Bmatrix}$$

- Sparsity, variable integral costs, algorithm constraints, symmetry, shell blocking, ...

Global Arrays (technologies)

Physically distributed data



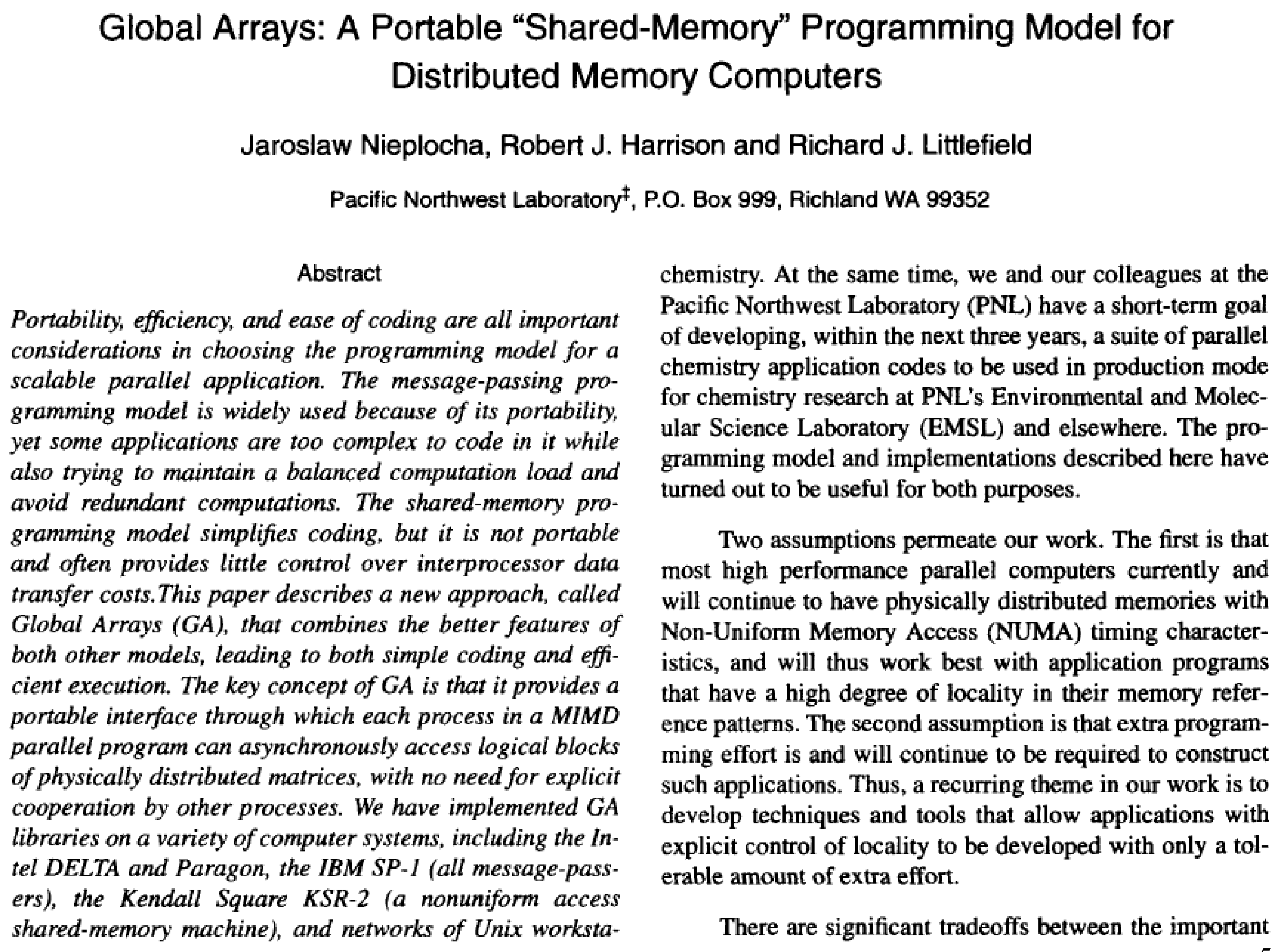
Single, shared data structure

- Shared-memory-like model
  - Fast local access
  - NUMA aware and easy to use
  - MIMD and data-parallel modes
  - Inter-operates with MPI, …
- BLAS and linear algebra interface
- Ported to major parallel machines
  - IBM, Cray, SGI, clusters,...
- Originated in an HPCC project
- Used by most major chemistry codes, financial futures forecasting, astrophysics, computer graphics
- Supported by DOE

- One of the legacies of Jarek Nieplocha, PNNL

http://www.emsl.pnl.gov/docs/global/

SC94



Global Arrays: A Portable "Shared-Memory" Programming Model for Distributed Memory Computers

Jaroslaw Nieplocha, Robert J. Harrison and Richard J. Littlefield

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Abstract

Portability, efficiency, and ease of coding are all important considerations in choosing the programming model for a scalable parallel application. The message-passing programming model is widely used because of its portability, yet some applications are too complex to code in it while also trying to maintain a balanced computation load and avoid redundant computations. The shared-memory programming model simplifies coding, but it is not portable and often provides little control over interprocessor data transfer costs.This paper describes a new approach, called Global Arrays (GA), that combines the better features of both other models, leading to both simple coding and efficient execution. The key concept of GA is that it provides a portable interface through which each process in a MIMD parallel program can asynchronously access logical blocks of physically distributed matrices, with no need for explicit cooperation by other processes. We have implemented GA libraries on a variety of computer systems, including the Intel DELTA and Paragon, the IBM SP-1 (all message-passers), the Kendall Square KSR-2 (a nonuniform access shared-memory machine), and networks of Unix worksta-

chemistry. At the same time, we and our colleagues at the Pacific Northwest Laboratory (PNL) have a short-term goal of developing, within the next three years, a suite of parallel chemistry application codes to be used in production mode for chemistry research at PNL's Environmental and Molecular Science Laboratory (EMSL) and elsewhere. The programming model and implementations described here have turned out to be useful for both purposes.

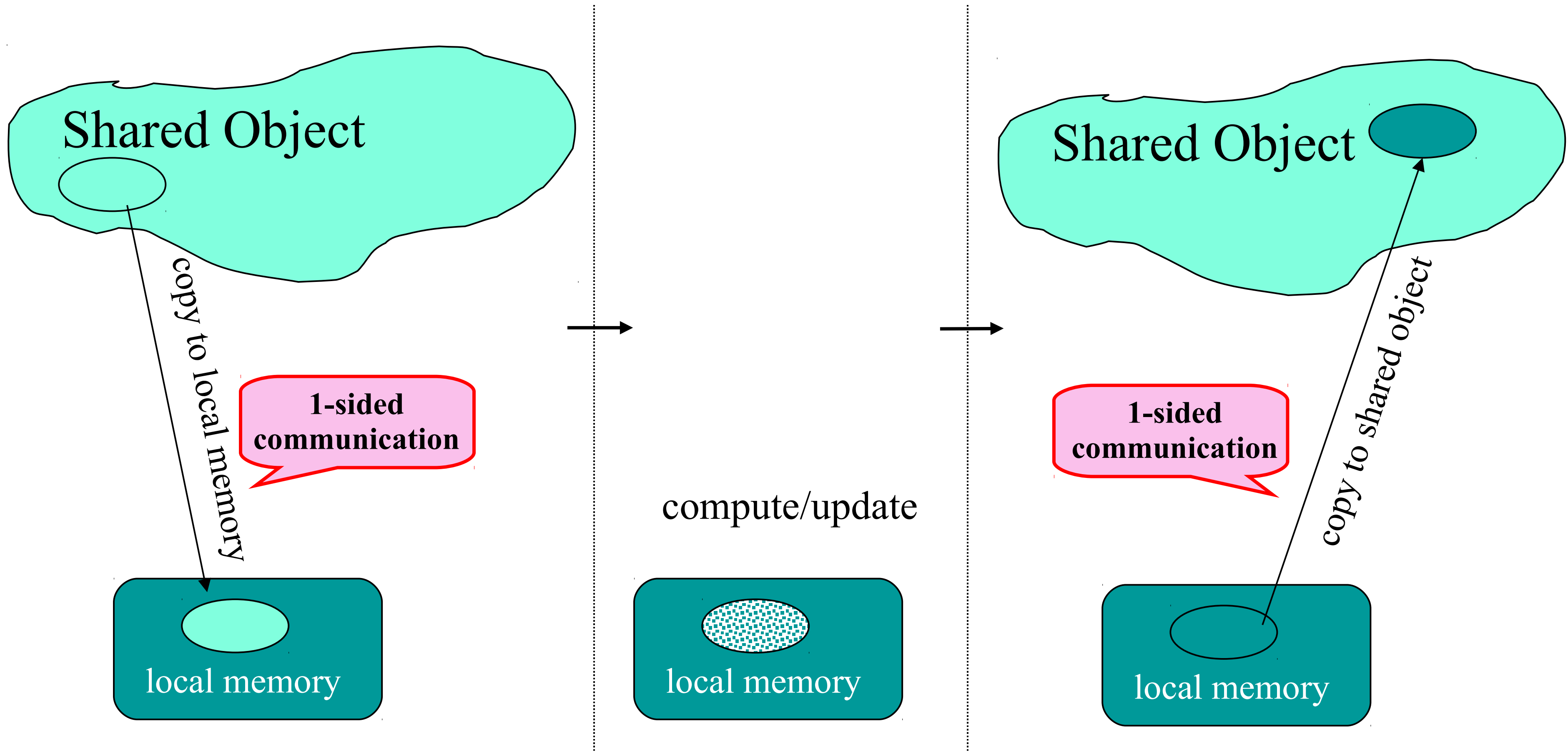
Two assumptions permeate our work. The first is that most high performance parallel computers currently and will continue to have physically distributed memories with Non-Uniform Memory Access (NUMA) timing characteristics, and will thus work best with application programs that have a high degree of locality in their memory reference patterns. The second assumption is that extra programming effort is and will continue to be required to construct such applications. Thus, a recurring theme in our work is to develop techniques and tools that allow applications with explicit control of locality to be developed with only a tolerable amount of extra effort.

There are significant tradeoffs between the important

History and Design

- Prototyping at very start of NWChem project
  - Model full application not just kernel
  - 80-20 rule – more like 90-10 rule
- GA designed to solve a problem
  - Distributing large data structures while supporting irregular computation
  - Entire HF code
  - First 2 attempts (Linda-like) worked for kernel but not the rest of the code

Non-uniform memory access model of computation

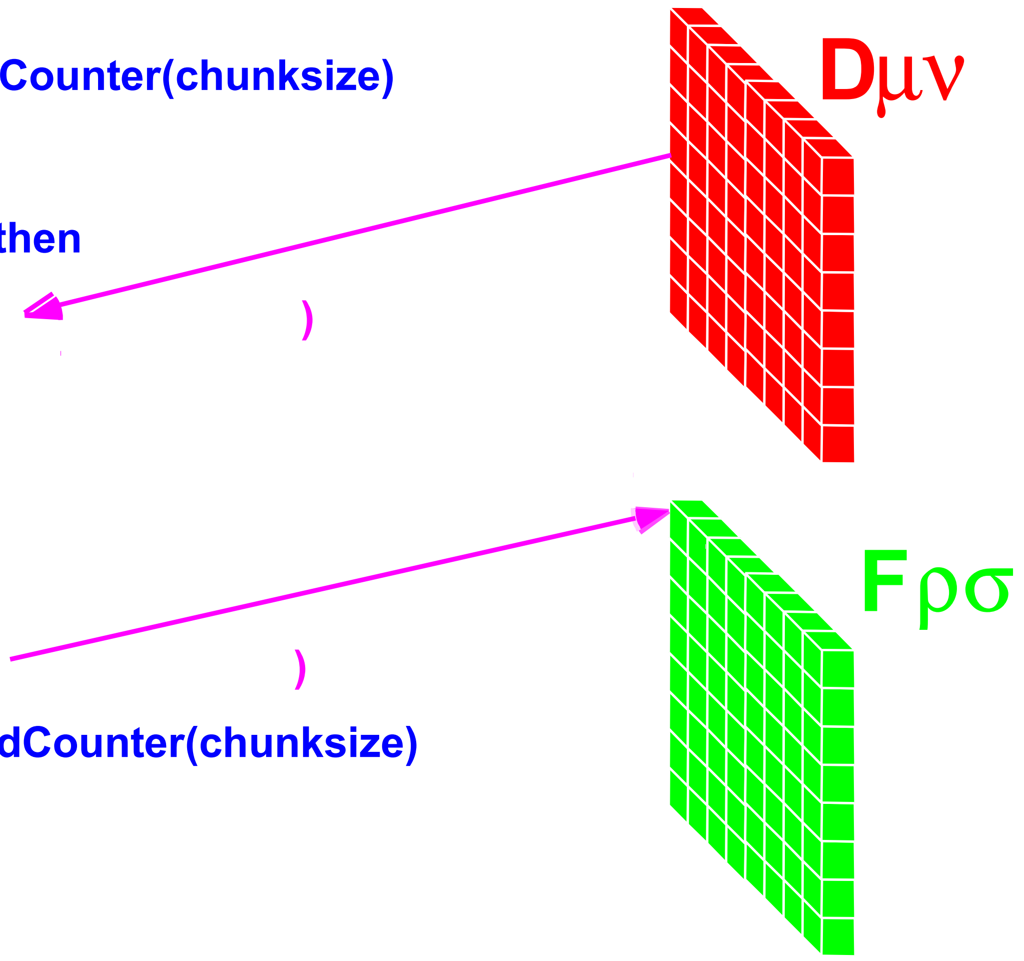


Dynamic load balancing

```
my_next_task = SharedCounter(chunksize)
do i=1,max_i
   if(i.eq.my_next_task) then
      call ga_get(                    )

            (do work)

      call ga_acc(                    )
     my_next_task = SharedCounter(chunksize)
     endif
enddo
Barrier()
```



Distributed data SCF

- First success for NWChem and Global Arrays

```
do tiles of i
    do tiles of j
        do tiles of k
            do tiles of l
                get patches ij, ik, il, jk, jl, kl
                compute integrals
                accumulate results back into patches
```

$\left.\begin{matrix} \text{do tiles of i} \\ \text{do tiles of j} \\ \text{do tiles of k} \\ \text{do tiles of l} \end{matrix}\right\}$ Parallel loop nest

Mini-apps used to evaluate HPCS languages Chapel, X10, Fortress
- just the data flow

B = block size

$t_{\text{comm}} = O(B^2)$ $\quad t_{\text{compute}} = O(B^4)$ $\quad \dfrac{t_{\text{compute}}}{t_{\text{comm}}} = O(B^2)$

Higher-performance code

- Looks nothing like that!
- Sort shell pairs to evaluate in similar batches
  - Precomputation, vectorization – 10-fold speedup
  - Big increase in complexity and memory use
- Integral evaluation code – 100K lines!
- Careful screening with rigorous inequalities
  - Robustness, minimize overhead

Highest-performance code

- Looks nothing like that!
- Strives for near linear scaling
- Coulomb interaction
  - Mix of FMM, FFT, and other fast methods
  - (near) linear scaling with system size
- Exchange interaction
  - Heavy screening and physical thresholding
- And this is just 1% of NWChem functionality

MADNESS

Multiresolution
Adaptive
Numerical
Scientific
Simulation

Multiresolution Adaptive Numerical Scientific Simulation

Robert J. Harrison[1], Scott Thornton[1], George I. Fann[2], Diego Galindo[2], Judy Hill[2], Jun Jia[2], Gregory Beylkin[4], Lucas Monzon[4], Hideo Sekino[5] Edward Valeev[6], Jeff Hammond[7], Nichols Romero[7], Alvaro Vasquez[7]

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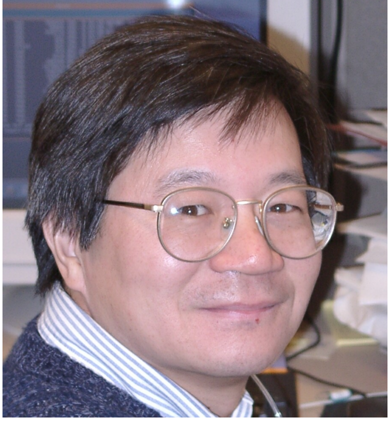

George Fann

Judy Hill

Gregory Beylkin

Rebecca Hartman-Baker

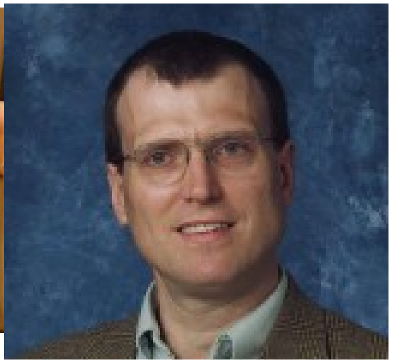
Jeff Hammond

Ariana Beste

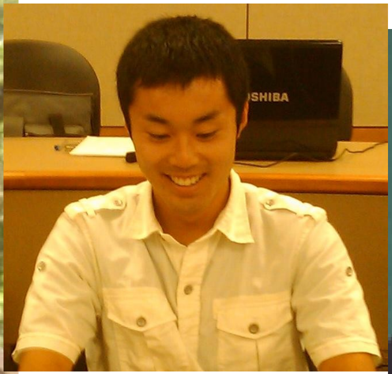
Eduard Valeyev

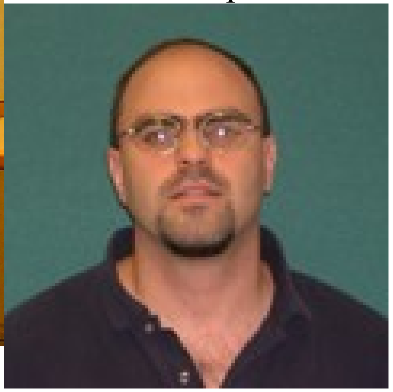
Alvaro Vasquez

Hideo Sekino


Robert Harrison

Nicholas Vence


Takahiro Ii


Scott Thornton

Matt Reuter

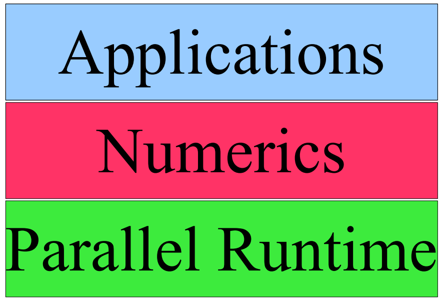
Nichols Romero

Jia, Kato, Calvin, Pei, ...

What is MADNESS?

- A general purpose numerical environment for reliable and fast scientific simulation
  - Chemistry, nuclear physics, atomic physics, material science, nanoscience, climate, fusion, ...
- A general purpose parallel programming environment designed for the peta/exa-scales
- Addresses many of the sources of complexity that constrain our HPC ambitions

http://code.google.com/p/m-a-d-n-e-s-s
http://harrison2.chem.utk.edu/~rjh/madness/



Why MADNESS?

- Reduces S/W complexity
  - MATLAB-like level of composition of scientific problems with guaranteed speed and precision
  - Programmer not responsible for managing dependencies, scheduling, or placement

- Reduces numerical complexity
  - Solution of integral not differential equations
  - Framework makes latest techniques in applied math and physics available to wide audience

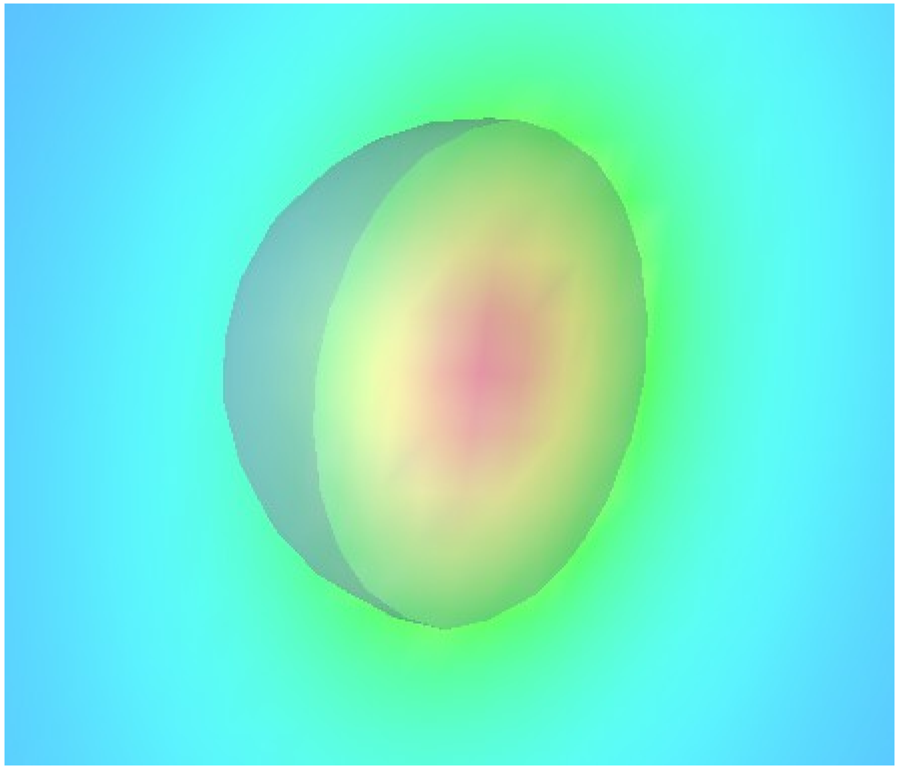
Big picture

- Want robust algorithms that scale correctly with system size and are easy to write
- Robust, accurate, fast computation
  - Gaussian basis sets: high accuracy yields dense matrices and linear dependence – $O(N^3)$
  - Plane waves: force pseudo-potentials – $O(N^3)$
  - $O(N \log^m N \log^k \varepsilon)$ is possible, guaranteed ε
- Semantic gap
  - Why are our equations just O(100) lines but programs O(1M) lines?
- Facile path from laptop to exaflop

E.g., with guaranteed precision of 1e-6 form a numerical representation of a Gaussian in the cube $[-20,20]^3$, solve Poisson's equation, and plot the resulting potential (all running in parallel with threads+MPI)

```
Let
    Ω = [−20, 20]^3
    ε = 1e − 6
    g = x → exp(−(x_0^2 + x_1^2 + x_2^2)) ∗ π^{−1.5}
In
    f = 𝓕 g
    u = ∇^{−2}(−4 ∗ π ∗ f)
    print "norm of f", ⟨f⟩, "energy", ⟨f|u⟩ ∗ 0.5
    plot u
End
```

output: norm of f 1.00000000e+00 energy 3.98920526e-01



There are only two lines doing real work. First the Gaussian (g) is projected into the adaptive basis to the default precision. Second, the Green's function is applied. The exact results are norm=1.0 and energy=0.3989422804.

He atom Hartree-Fock

```
Let
  $\Omega = [-20, 20]^3$
  $r = x \to \sqrt{x_0^2 + x_1^2 + x_2^2}$
  $g = x \to \exp\left(-2 * r(x)\right)$
  $v = x \to -\frac{2}{r(x)}$
In
  $\nu = \mathcal{F}\ v$
  $\phi = \mathcal{F}\ g$
  $\lambda = -1.0$
  for $i \in [0, 10]$
    $\phi = \phi * \|\phi\|^{-1}$
    $V = \nu - \nabla^{-2}\left(4 * \pi * \phi^2\right)$
    $\psi = -2 * \left(-2 * \lambda - \nabla^2\right)^{-1}(V * \phi)$
    $\lambda = \lambda + \frac{\langle V * \phi | \psi - \phi \rangle}{\langle \psi | \psi \rangle}$
    $\phi = \psi$
    print "iter", $i$, "norm", $\|\phi\|$, "eval", $\lambda$
  end
End
```

Compose directly in terms of functions and operators

This is a Latex rendering of a program to solve the Hartree-Fock equations for the helium atom

The compiler also output a C++ code that can be compiled without modification and run in parallel

“Fast” algorithms

- Fast in mathematical sense
  - Optimal scaling of cost with accuracy & size
- Multigrid method – Brandt (1977)
  - Iterative solution of differential equations
  - Analyzes solution/error at different length scales
- Fast multipole method – Greengard, Rokhlin (1987)
  - Fast application of dense operators
  - Exploits smoothness of operators
- Multiresolution analysis
  - Exploits smoothness of operators and functions

The math behind the MADNESS

- Multiresolution

$$V_0 \subset V_1 \subset \cdots \subset V_n$$

$$V_n = V_0 + \left(V_1 - V_0\right) + \cdots + \left(V_n - V_{n-1}\right)$$

- Low-separation rank

$$f(x_{1,} \ldots, x_n) = \sum_{l=1}^{M} \sigma_l \prod_{i=1}^{d} f_i^{(l)}(x_i) + O(\epsilon)$$

$$\left\| f_i^{(l)} \right\|_2 = 1 \qquad \sigma_l > 0$$

- Low-operator rank

$$A = \sum_{\mu=1}^{r} u_\mu \sigma_\mu v_\mu^T + O(\epsilon)$$

$$\sigma_\mu > 0 \qquad v_\mu^T v_\lambda = u_\mu^T u_\lambda = \delta_{\mu\nu}$$

Why “think” multiresolution?

- It is everywhere in nature/chemistry/physics
  - Core/valence; high/low frequency; short/long range; smooth/non-smooth; atomic/nano/micro/macro scale
- Common to separate just two scales
  - E.g., core orbital heavily contracted, valence flexible
  - More efficient, compact, and numerically stable
- Multiresolution
  - Recursively separate all length/time scales
  - Computationally efficient and numerically stable
  - Coarse-scale models that capture fine-scale detail

How to “think” multiresolution

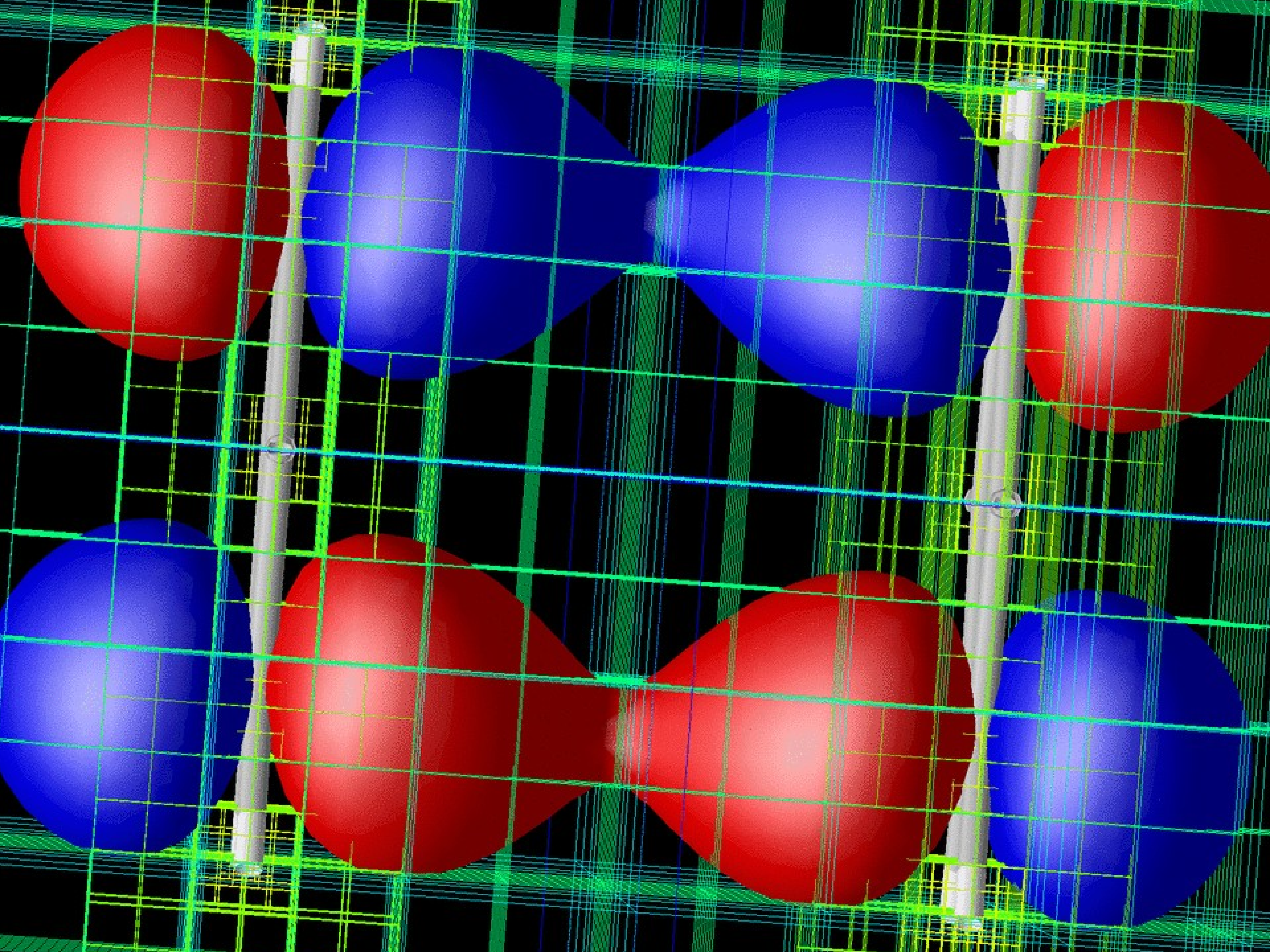
- Consider a ladder of function spaces

$$V_0 \subset V_1 \subset \cdots \subset V_n$$

  - E.g., increasing quality atomic basis sets, or finer resolution grids, …
- Telescoping series

$$V_n = V_0 + \left(V_1 - V_0\right) + \cdots + \left(V_n - V_{n-1}\right)$$

  - Instead of using the most accurate representation, use the difference between successive approximations
  - Representation on V_0 small/dense; differences sparse
  - Computationally efficient; possible insights

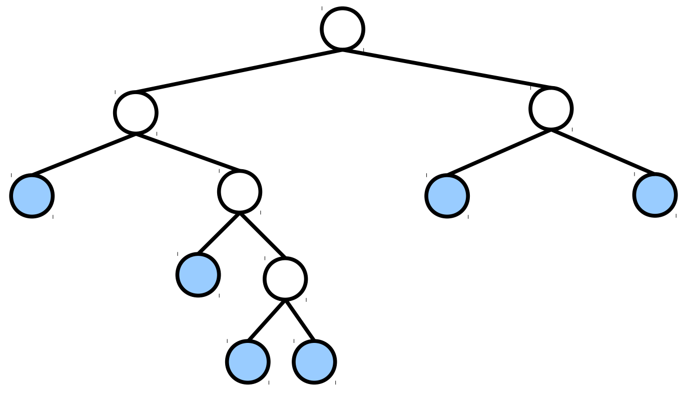


Another Key Component

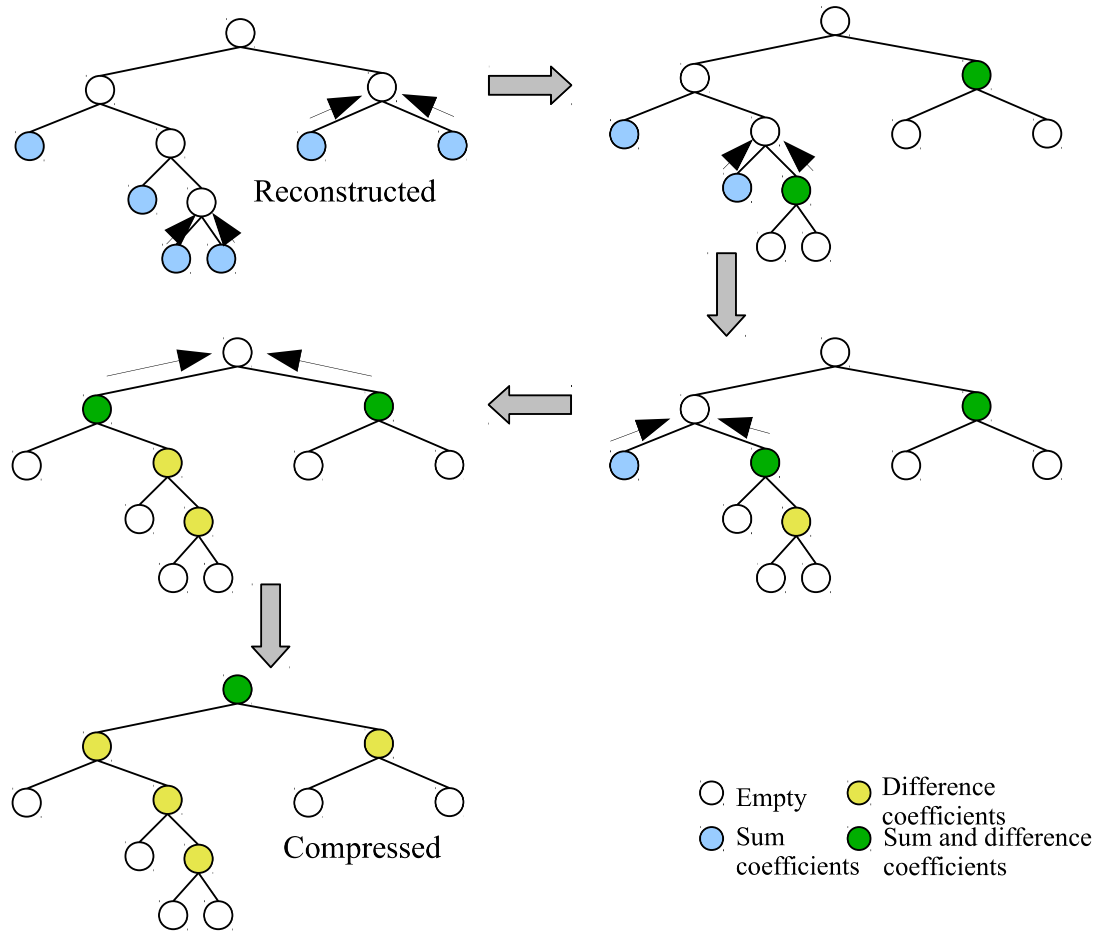
- Trade precision for speed – everywhere
  - Don’t do anything exactly
  - Perform everything to $O(\varepsilon)$
  - Require
    - Robustness
    - Speed, and
    - Guaranteed, arbitrary, *finite* precision

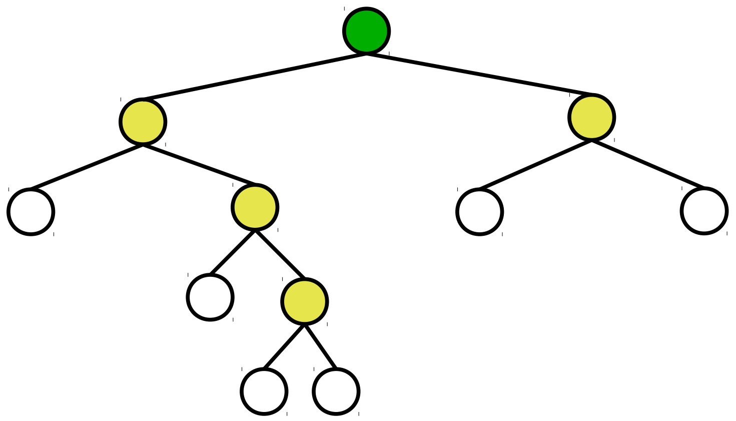
Please forget about wavelets

- They are not central
- Wavelets are a convenient basis for spanning V_n-V_{n-1} and understanding its properties
- But you don't actually need to use them
  - MADNESS does still compute wavelet coefficients, but *Beylkin's new code does not*
- Please remember this …
  - Discontinuous spectral element with multi-resolution and separated representations for fast computation with guaranteed precision in many dimensions.



Tree in **reconstructed** form. Scaling function (sum) coefficients at leaf nodes. Interior nodes empty.



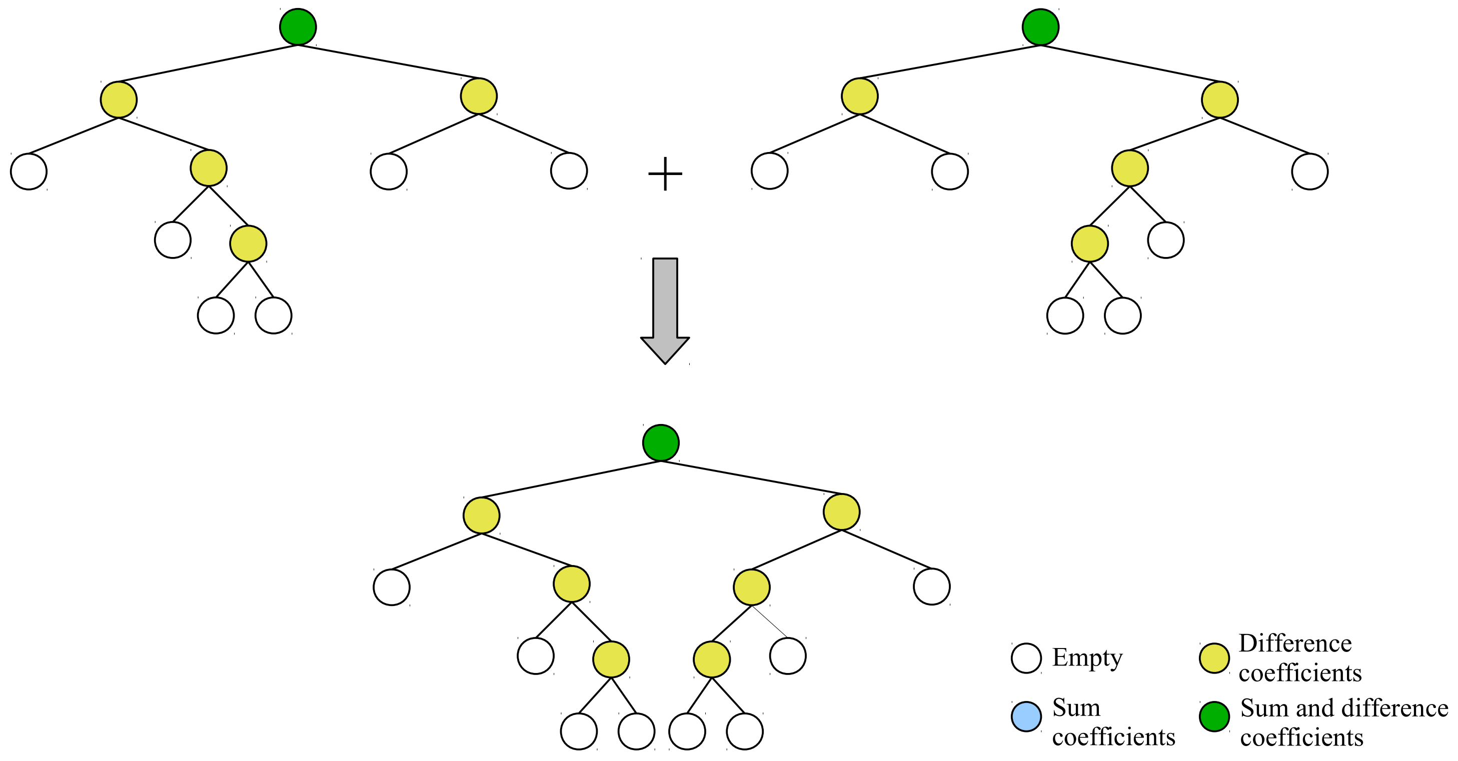


Tree in **compressed** form. Wavelet (difference) coefficients at interior nodes, with scaling functions coefficients also at root. Leaf nodes empty.

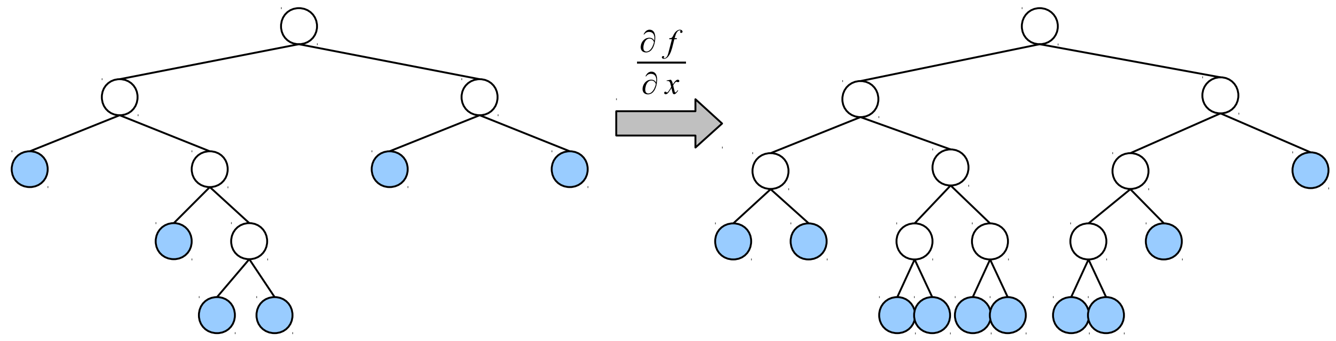
Compression algorithm. Starting from leaf nodes, scaling function (sum) coefficients are passed to parent. Parent "filters" the childrens' coefficients to produce sum and wavelet (difference) coefficients at that level, then passes sum coefficients to its parent.

Reconstruction is simply the reverse processes.

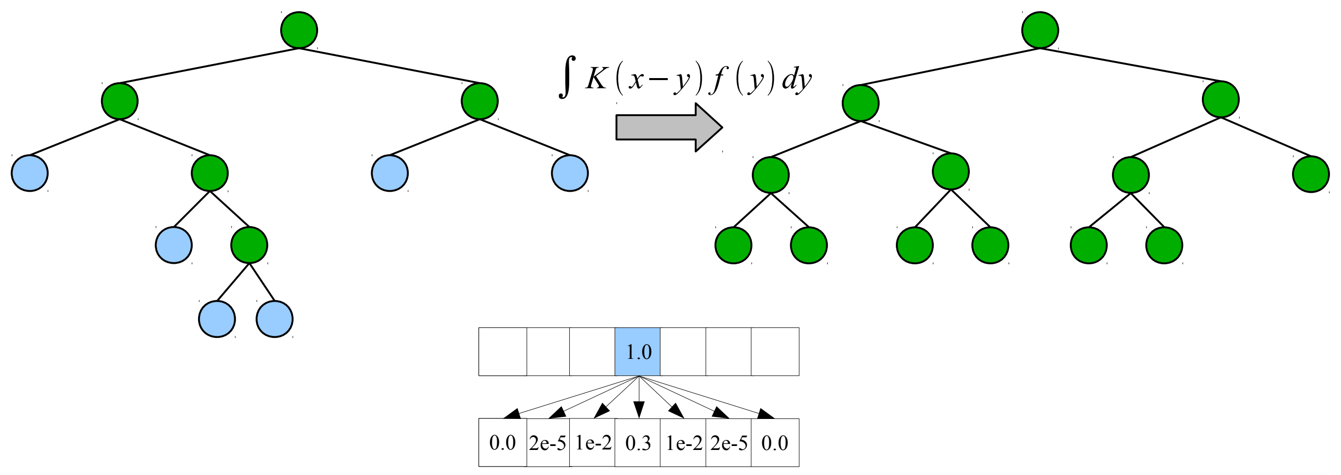
To produce the non-standard form the compression algorithm is run but scaling function coefficients are retained at the leaf and interior nodes.



Addition is (most straightforwardly) performed in the compressed form. Coefficients are simply added with missing nodes being treated as if zero.

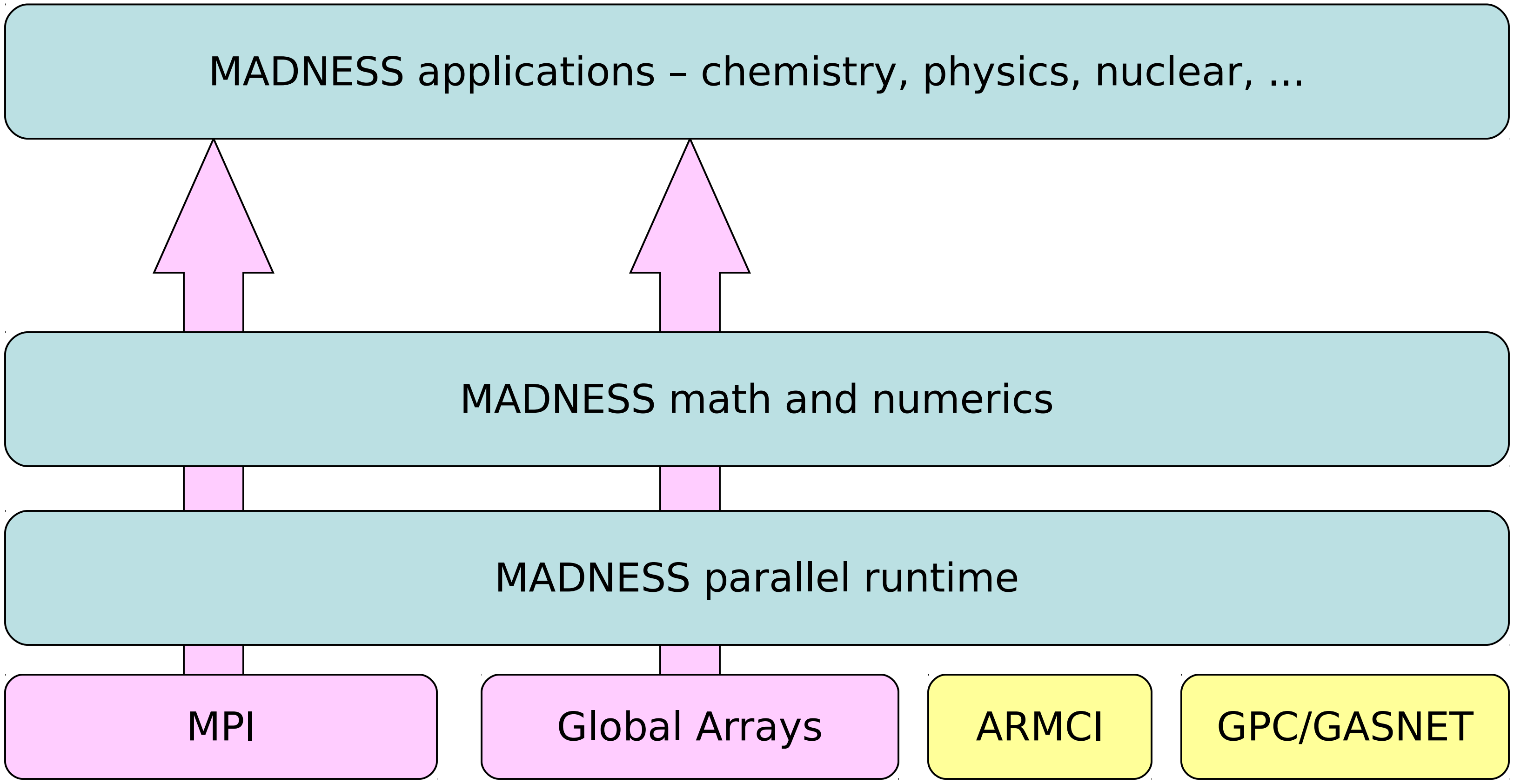


Differentiation (for simplicity here using central differences and Dirichlet boundary conditions) is applied in the scaling function basis. To compute the derivative of the function in the box corresponding to a leaf node, we require the coefficients from the neighboring boxes at the same level. If the neighboring leaf nodes exist, all is easy. If it exists at a higher level,we can make the coefficients using the two-scale relation. But if the neighbor exists at a finer scale, we must recur down until both neighbors are at the same level. Hence, phrased as parallel computation on all leaf nodes , differentiation must search for neighbors in the tree at the same and higher levels, and may initiate computation at lower levels. It can also be phrased as a recursive descent of the tree, which can have advantages in reducing the amount of probes up the tree for parents of neighbors (esp. in higher dimensions).



Convolution with a function is applied in the non-standard form, thus the first step is to compress into non-standard form. Then we can independently compute the contribution of each box (node) to the result *at the same level of the tree*. Depending upon dimensionality, accuracy, and the kernel (*K*), we usually only need to compute the contributions of a box to itself and its immediate neighbors. The support (i.e., level of refinement) of the result is very dependent on the kernel. Here we consider convolution with a Gaussian (Green's function for the heat equation) which is a *smoothing* operator. After the computation is complete, we must sum down the tree to recover the standard form. Hence, phrased as computation on all the nodes in non-standard form, convolution requires compression and reconstruction, and during the computation communicates across the tree at the same level to add results into neighboring boxes and up the tree to connect new nodes to parents.

MADNESS architecture


MADNESS applications – chemistry, physics, nuclear, ...
MADNESS math and numerics
MADNESS parallel runtime
MPI
Global Arrays
ARMCI
GPC/GASNET

Intel Thread Building Blocks now the target for the intranode runtime

Runtime Objectives

- Scalability to 1+M processors ASAP
- Runtime responsible for
  - scheduling and placement,
  - managing dependencies & hiding latency
- Compatible with existing models (MPI, GA)
- Borrow successful concepts from Cilk, Charm++, Python, HPCS languages

Why a new runtime?

- MADNESS computation is irregular & dynamic
  - 1000s of dynamically-refined meshes changing frequently & independently (to guarantee precision)
- Because we wanted to make MADNESS itself easier to write not just the applications using it
  - We explored implementations with MPI, Global Arrays, and Charm++ and all were inadequate
- MADNESS is helping drive
  - One-sided operations in MPI-3, DOE projects in fault tolerance, ...

Key runtime elements

- Futures for hiding latency and automating dependency management
- Global names and name spaces
- Non-process centric computing
  - One-sided messaging between objects
  - Retain place=process for MPI/GA legacy compatibility
- Dynamic load balancing
  - Data redistribution, work stealing, randomization

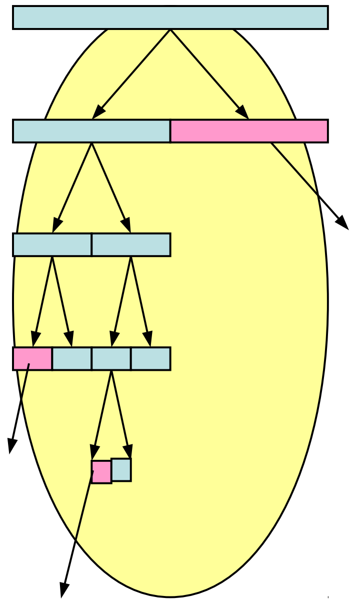
Futures

- Result of an asynchronous computation
  - Cilk, Java, HPCLs, C++0x
- Hide latency due to communication or computation
  -
- Management of dependencies
  - Via callbacks

```
int f(int arg);
ProcessId me, p;

Future<int> r0=task(p, f, 0);
Future<int> r1=task(me, f, r0);

// Work until need result

cout << r0 << r1 << endl;
```

Process “me” spawns a new task in process “p” to execute `f(0)` with the result eventually returned as the value of future `r0`. This is used as the argument of a second task whose execution is deferred until its argument is assigned. Tasks and futures can register multiple local or remote callbacks to express complex and dynamic dependencies.

Virtualization of data and tasks



Future:
- MPI rank
- probe()
- set()
- get()

Task:
- Input parameters
- Output parameters
- probe()
- run()
- get()

```
Future Compress(tree):
      Future left = Compress(tree.left)
      Future right = Compress(tree.right)
      return Task(Op, left, right)

Compress(tree)
Wait for all tasks to complete
```

Benefits: Communication latency & transfer time largely hidden
Much simpler composition than explicit message passing
Positions code to use "intelligent" runtimes with work stealing
Positions code for efficient use of multi-core chips
Locality-aware and/or graph-based scheduling

Global Names

- Objects with global names with different state in each process
  - C.f. shared[threads] in UPC; co-Array
- Non-collective constructor; deferred destructor
  - Eliminates synchronization

```
class A : public WorldObject<A>
{
   int f(int);
};
ProcessID p;
A a(world);
Future<int> b =
   a.task(p,&A::f,0);
```

A task is sent to the instance of a in process p. If this has not yet been constructed the message is stored in a pending queue. Destruction of a global object is deferred until the next user synchronization point.

```
#define WORLD_INSTANTIATE_STATIC_TEMPLATES
#include <world/world.h>
using namespace madness;
class Foo : public WorldObject<Foo> {
    const int bar;
public:
    Foo(World& world, int bar) : WorldObject<Foo>(world), bar(bar)
                {process_pending();}

    int get() const {return bar;}
};
int main(int argc, char** argv) {
    MPI::Init(argc, argv);
    madness::World world(MPI::COMM_WORLD);

    Foo a(world,world.rank()), b(world,world.rank()*10)

    for (ProcessID p=0; p<world.size(); p++) {
        Future<int> futa = a.send(p,&Foo::get);
        Future<int> futb = b.send(p,&Foo::get);
        // Could work here until the results are available
        MADNESS_ASSERT(futa.get() == p);
        MADNESS_ASSERT(futb.get() == p*10);
    }
    world.gop.fence();
    if (world.rank() == 0) print("OK!");
    MPI::Finalize();
}
```

Figure 1: Simple client-server program implemented using WorldObject.

```
#define WORLD_INSTANTIATE_STATIC_TEMPLATES
#include <world/world.h>

using namespace std;
using namespace madness;

class Array : public WorldObject<Array> {
   vector<double> v;
public:
   /// Make block distributed array with size elements
   Array(World& world, size_t size)
      : WorldObject<Array>(world), v((size-1)/world.size()+1)
   {
      process_pending();
   };

   /// Return the process in which element i resides
   ProcessID owner(size_t i) const {return i/v.size();};

   Future<double> read(size_t i) const {
      if (owner(i) == world.rank())
         return Future<double>(v[i-world.rank()*v.size()]);
      else
         return send(owner(i), &Array::read, i);
   };

   Void write(size_t i, double value) {
      if (owner(i) == world.rank())
         v[i-world.rank()*v.size()] = value;
      else
         send(owner(i), &Array::write, i, value);
      return None;
   };
};
```

```
int main(int argc, char** argv) {
   initialize(argc, argv);
   madness::World world(MPI::COMM_WORLD);

   Array a(world, 10000), b(world, 10000);

   // Without regard to locality, initialize a and b
   for (int i=world.rank(); i<10000; i+=world.size()) {
      a.write(i, 10.0*i);
      b.write(i,  7.0*i);
   }
   world.gop.fence();

   // All processes verify 100 random values from each array
   for (int j=0; j<100; j++) {
      size_t i = world.rand()%10000;
      Future<double> vala = a.read(i);
      Future<double> valb = b.read(i);
      // Could do work here until results are available
      MADNESS_ASSERT(vala.get() == 10.0*i);
      MADNESS_ASSERT(valb.get() ==  7.0*i);
   }
   world.gop.fence();

   if (world.rank() == 0) print("OK!");
   finalize();
}
```

Complete example program illustrating the implementation and use of a crude, block-distributed array upon the functionality of `WorldObject`.

Global Namespaces

- Specialize global names to containers
  - Hash table, arrays, ...
- Replace global pointer (process+local pointer) with more powerful concept
- User definable map from keys to "owner" process

```
class Index;   // Hashable
class Value {
   double f(int);
};

WorldContainer<Index,Value> c;
Index i,j;  Value v;
c.insert(i,v);
Future<double> r =
   c.task(j,&Value::f,666);
```

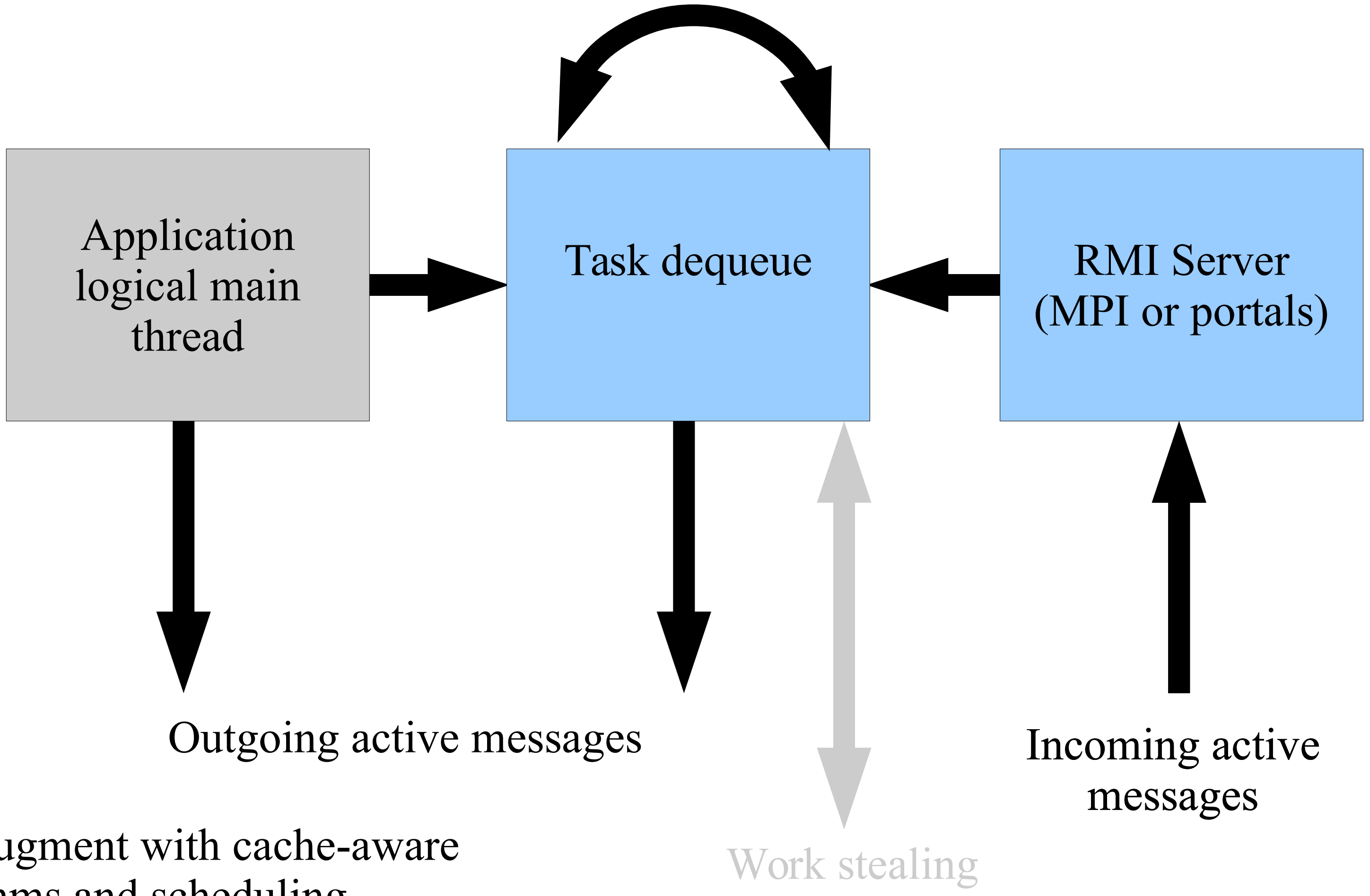
A container is created mapping indices to values.

A value is inserted into the container.

A task is spawned in the process owning key `j` to invoke `c[j].f(666)`.

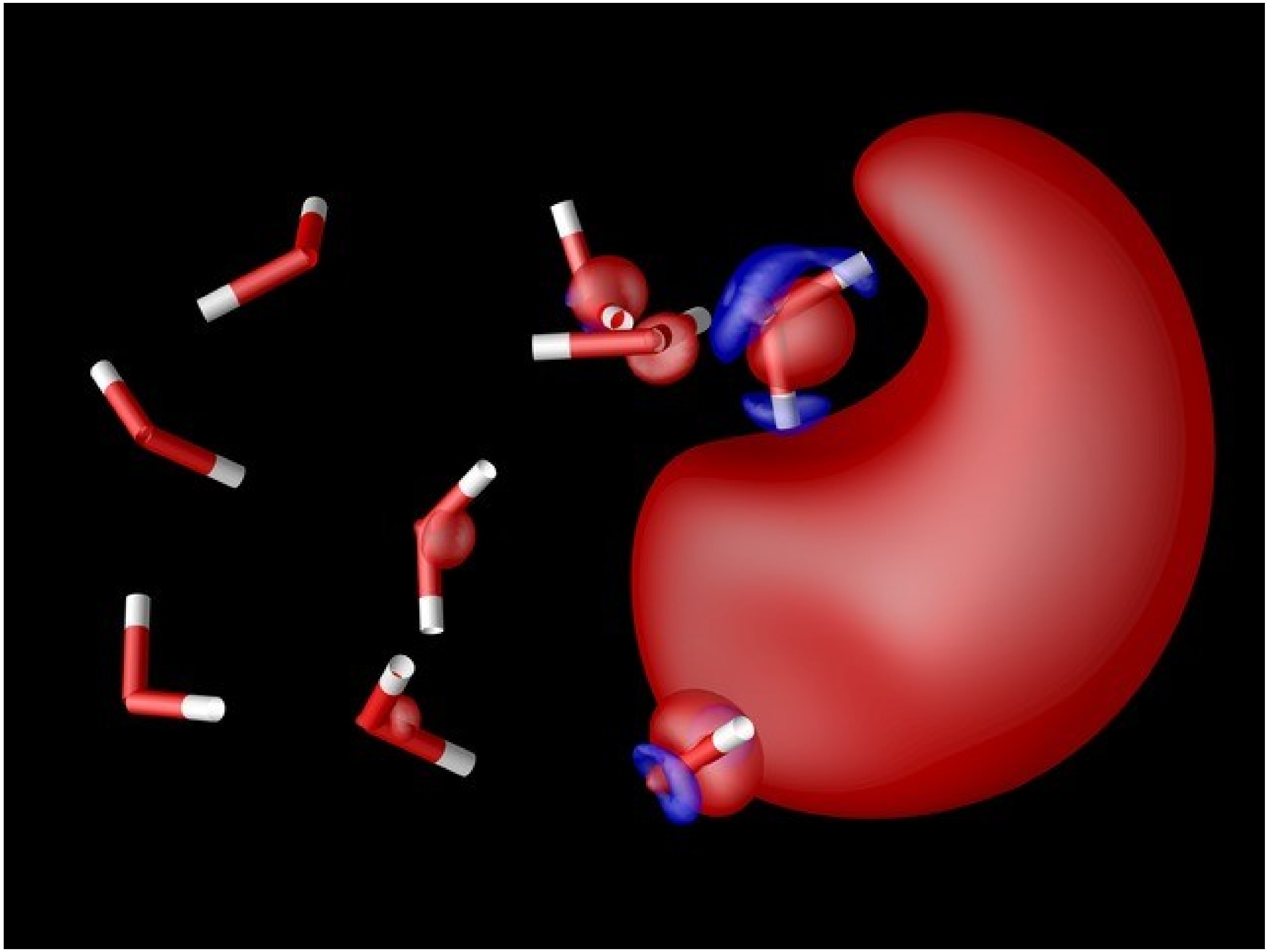
Namespaces are a large part of the elegance of Python and success of Charm++ (chares+arrays)

Multi-threaded architecture



Must augment with cache-aware algorithms and scheduling

Molecular Electronic Structure



Energy and gradients

ECPs coming (Sekino, Thornton)

Response properties (Vasquez, Yokoi, Sekino)

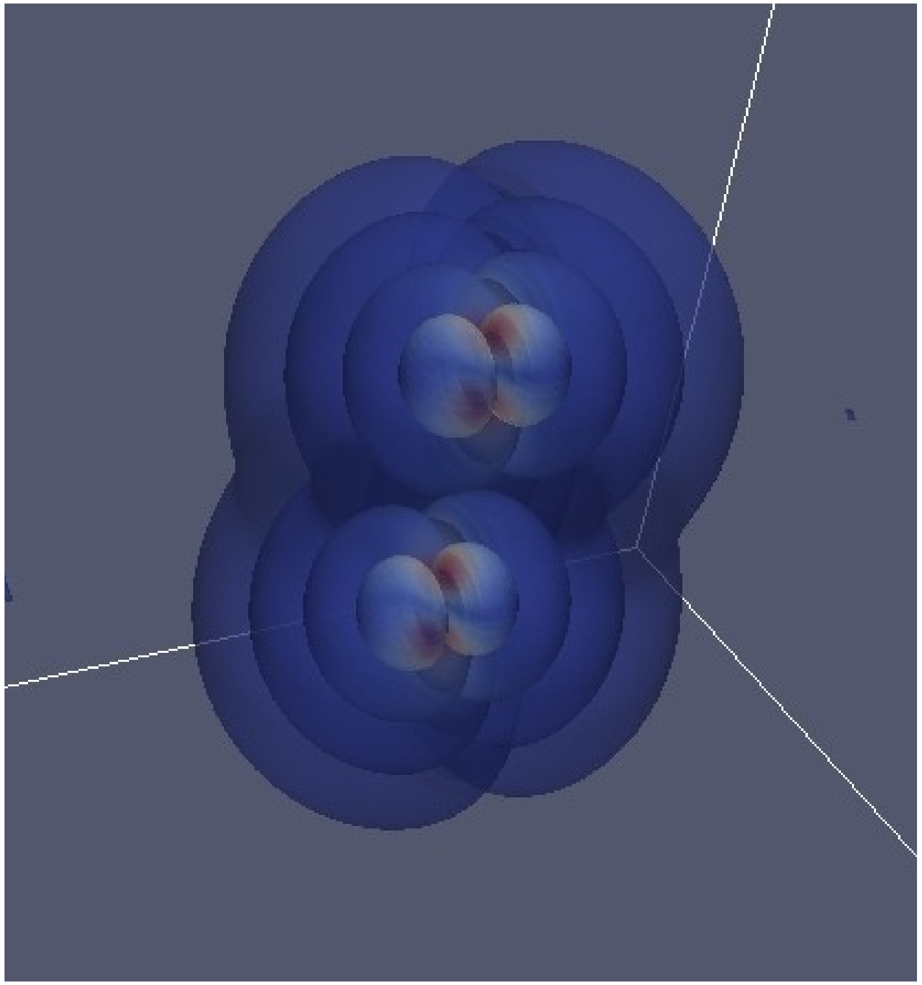
Still not as functional as previous Python version of Yanai

Spin density of solvated electron

Nuclear physics

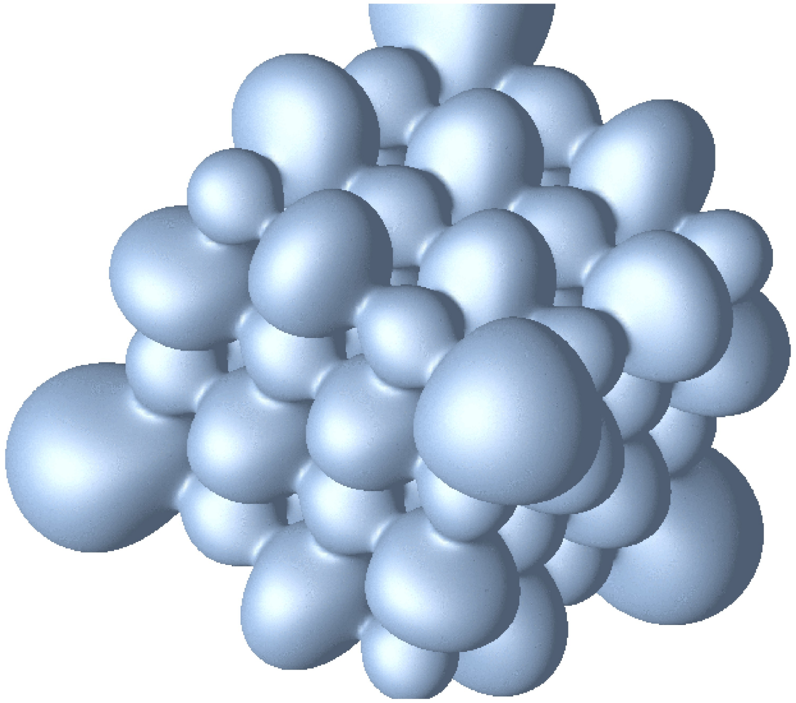
J. Pei, G.I. Fann, Y. Ou,
W. Nazarewicz
UT/ORNL

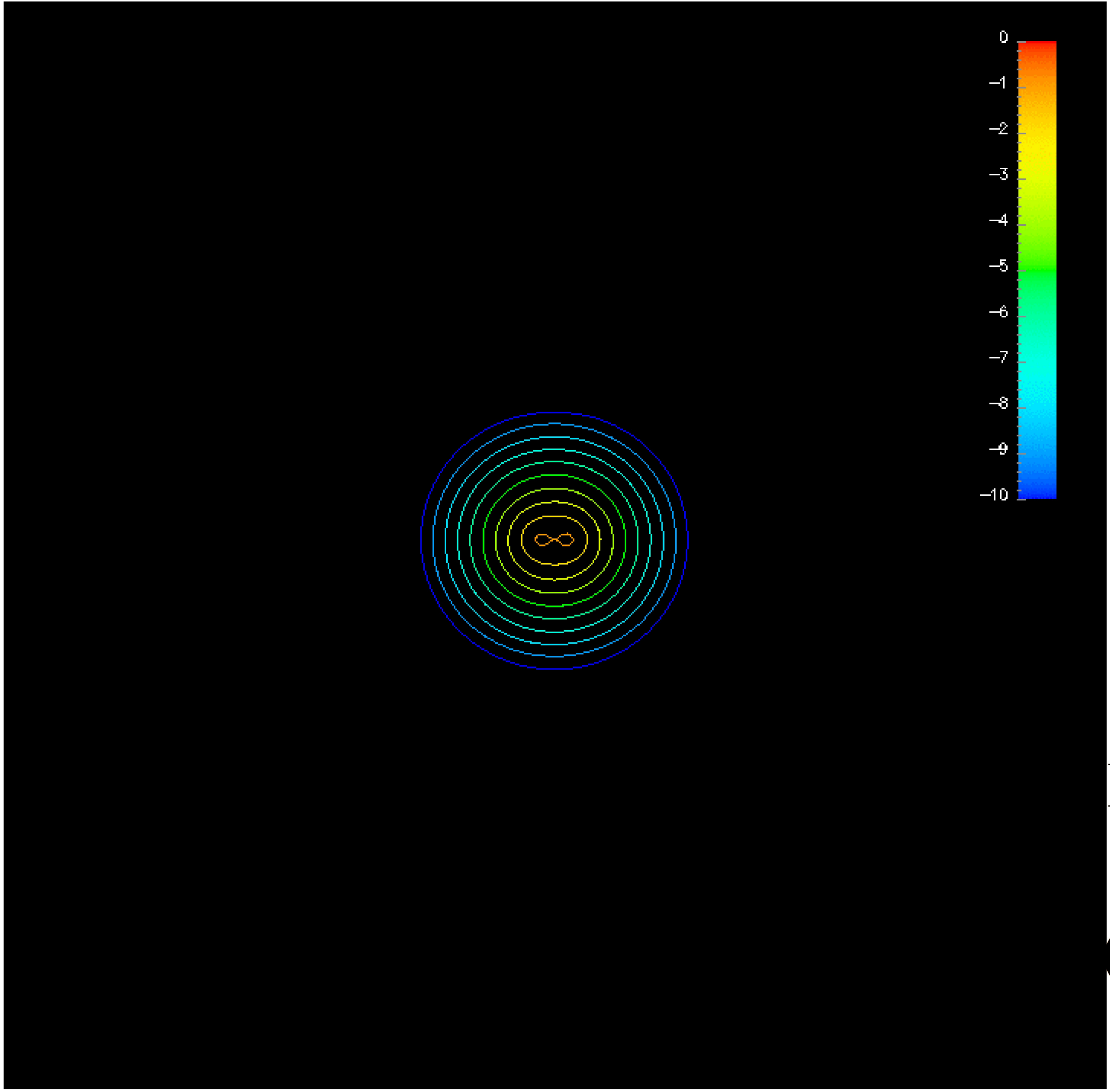
- DOE UNDEF
- Nuclei & neutron matter
- ASLDA
- Hartree-Fock Bogliobulov
- Spinors
- Gamov states


Imaginary part of the seventh eigen function
two-well Wood-Saxon potential

Solid-state electronic structure

- Thornton, Eguiluz and Harrison (UT/ORNL)
  - NSF OCI-0904972: Computational chemistry and physics beyond the petascale
- Full band structure with LDA and HF for periodic systems
- In development: hybrid functionals, response theory, post-DFT methods such as GW and model many-body Hamiltonians via Wannier functions


Coulomb potential isosurface in LiF



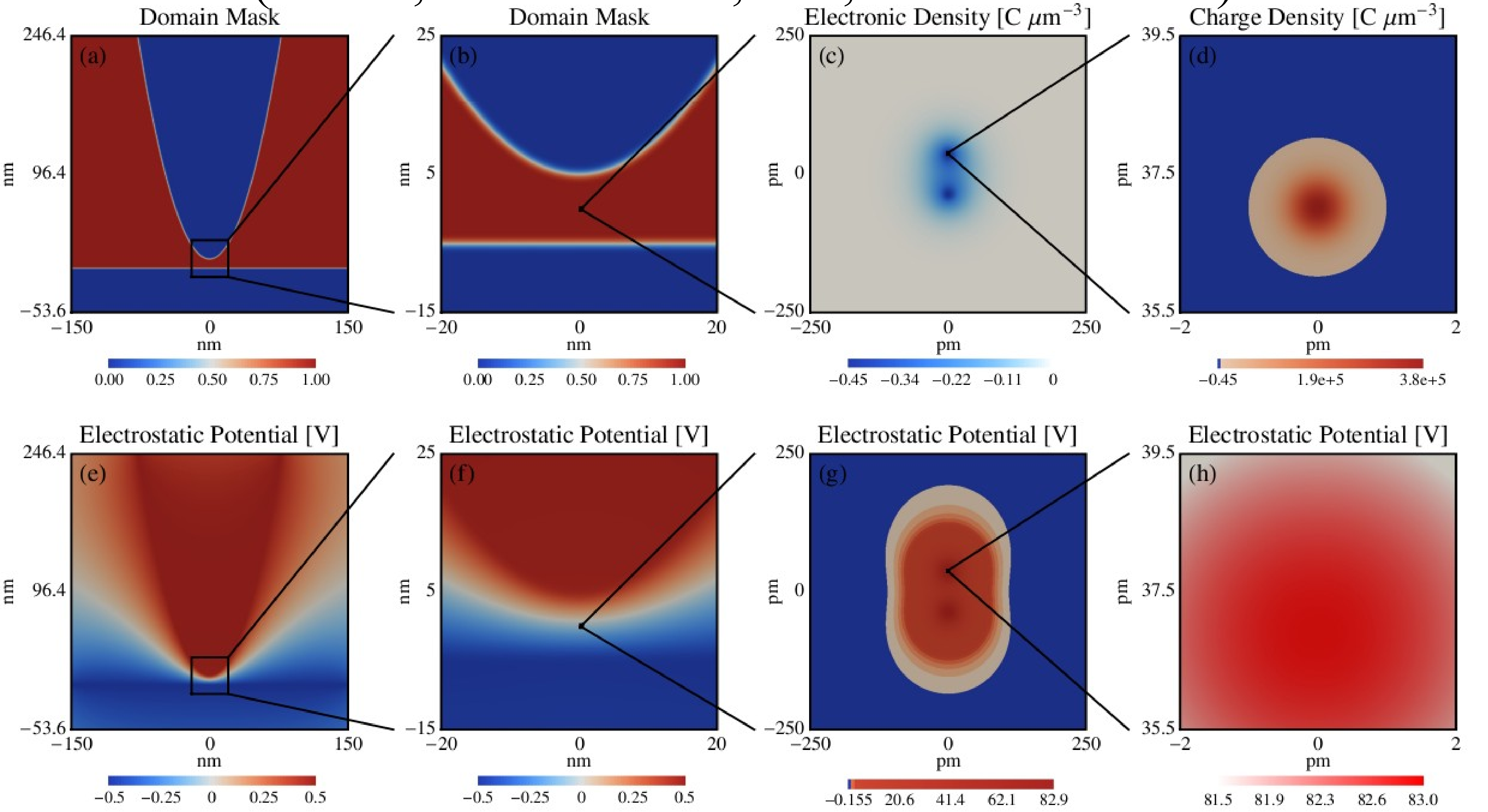
Time dependent electronic structure

Vence, Krstic, Harrison UT/ORNL

H_2^+ molecule in laser field (fixed nuclei)

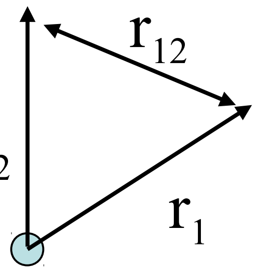
Nanoscale photonics

(Reuter, Northwestern; Hill, Harrison ORNL)



Diffuse domain approximation for interior boundary value problem; long-wavelength Maxwell equations; Poisson equation; Micron-scale Au tip 2 nm above Si surface with H2 molecule in gap – 10^7 difference betwee
shortest and longest length scales.

Electron correlation (6D)



- All defects in mean-field model are ascribed to electron correlation
- Singularities in Hamiltonian imply for a two-electron atom

$$\Psi(r_1, r_2, r_{12}) = 1 + \frac{1}{2} r_{12} + \cdots \quad \text{as} \quad r_{12} \to 0$$

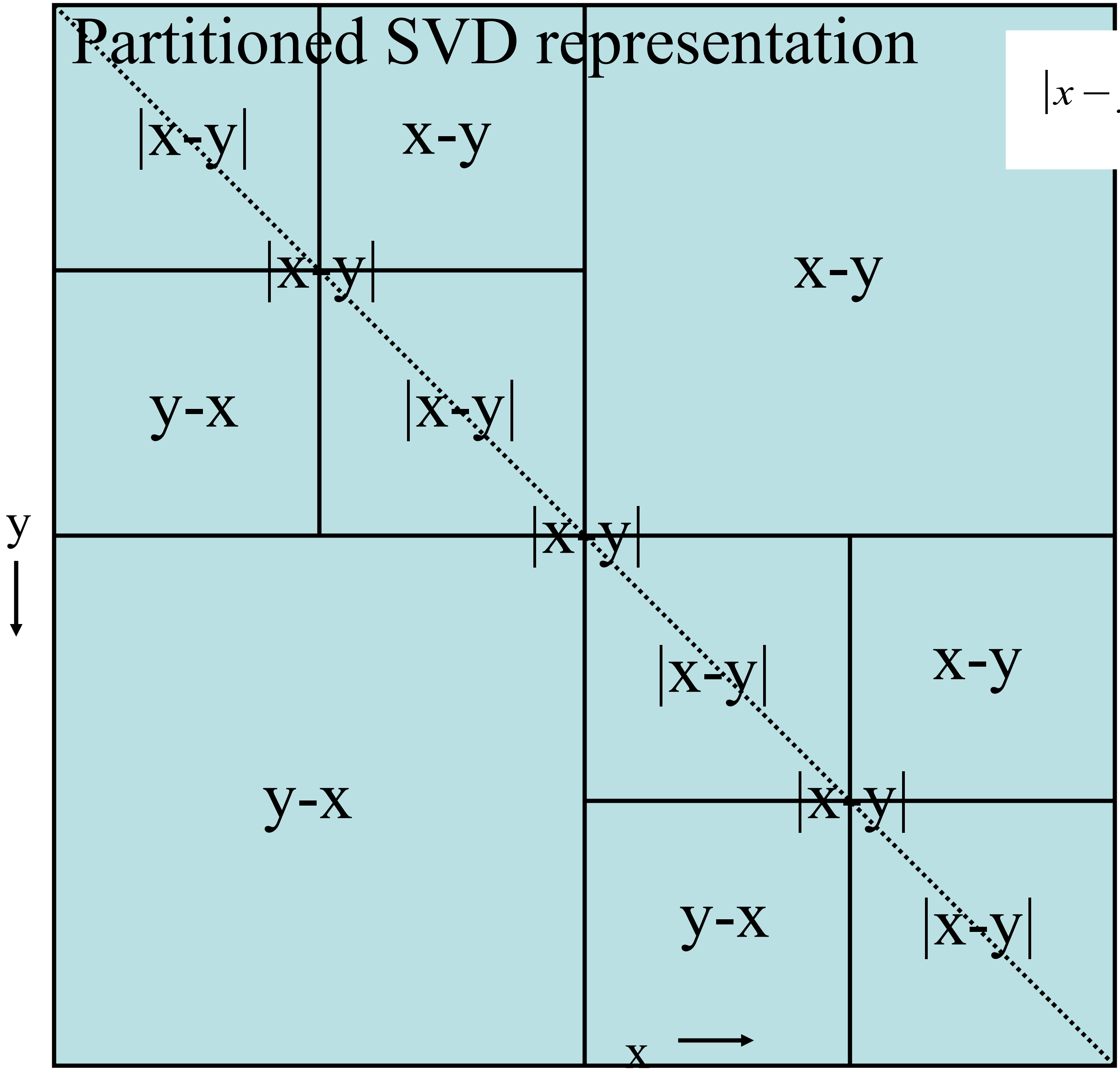
- Include the inter-electron distance in the wavefunction
  - E.g., Hylleraas 1938 wavefunction for He

$$\Psi(r_1, r_2, r_{12}) = \exp(-\xi(r_1 + r_2))(1 + a r_{12} + \cdots)$$

  - Potentially very accurate, but not systematically improvable, and (until recently) not computationally feasible for many-electron systems
- Configuration interaction expansion – slowly convergent

$$\Psi(r_1, r_2, \ldots) = \sum_i c_i \left| \phi_1^{(i)}(r_1) \phi_2^{(i)}(r_2) \ldots \right|$$

Partitioned SVD representation



$$|x-y| = \sum_{\mu=1}^{r} f_{\mu}(x) g_{\mu}(y)$$

r = separation rank

In 3D, ideally must be one box removed from the diagonal

Diagonal box has full rank

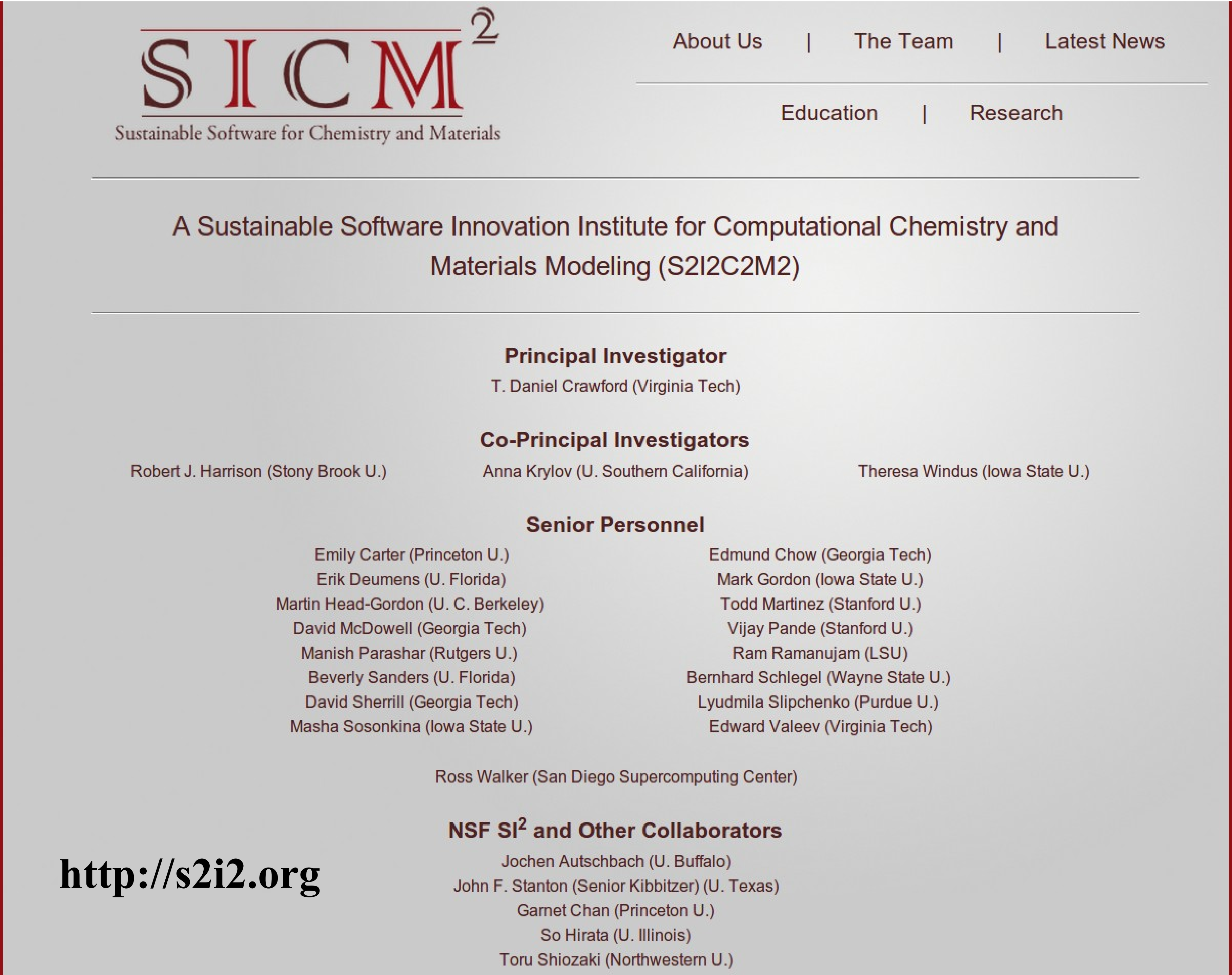
Boxes touching diagonal (face, edge, or corner) have increasingly low rank

Away from diagonal $r = O(-\log \varepsilon)$

The way forward demands a change in paradigm

- by us chemists, the funding agencies, and the supercomputer centers

- A communal effort recognizing the increased cost and complexity of code development for modern theory beyond the petascale
- Coordination between agencies to develop and deploy new simulation capabilities in sustainable manner
- Re-emphasizing basic and advanced theory and computational skills in undergraduate and graduate education



SICM^2

Sustainable Software for Chemistry and Materials

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http://s2i2.org

Summary

- We need radical changes in how we compose scientific S/W
  - Complexity at limits of cost and human ability
  - Need extensible tools/languages with support for code transformation not just translation
- Students need to be prepared for computing and data in 2020+ not as it was in 2000 and before
  - Pervasive, massive parallelism
  - Bandwidth limited computation and analysis
  - An intrinsically multidisciplinary activity

Stony Brook University

iACS INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

Funding

- DOE: Exascale co-design, SciDAC, Office of Science divisions of Advanced Scientific Computing Research and Basic Energy Science, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, in part using the National Center for Computational Sciences.
- DARPA HPCS2: HPCS programming language evaluation
- NSF CHE-0625598: Cyber-infrastructure and Research Facilities: Chemical Computations on Future High-end Computers
- NSF CNS-0509410: CAS-AES: An integrated framework for compile-time/run-time support for multi-scale applications on high-end systems
- NSF OCI-0904972: Computational Chemistry and Physics Beyond the Petascale

Problem with Differential Form

- Consider application of the Laplacian to a function with high-frequency numerical noise

$$\nabla^2\left(f(\boldsymbol{r})+\epsilon e^{i\boldsymbol{k}.r}\right)=\nabla^2 f(\boldsymbol{r})-k^2\epsilon e^{i\boldsymbol{k}.r}$$

- Consider 30 levels of adaptive refinement (and don't forget discontinuities, polynomials)

$$|k|\approx 10^9 \qquad k^2\approx 10^{18}$$

- I.e., we just took numerical noise $O\left(10^{-16}\right)$and amplified it to *O(100)*

Advantages of Integral Form

- Condition number of inverse Laplacian just as bad (unbounded spectrum & zero eigenvalues)
  - But for the inverse, large eigenvalues correspond to the smooth and usually interesting bits

$$\nabla^{-2}\left(f\left(\boldsymbol{r}\right)+\epsilon e^{i\boldsymbol{k}.r}\right)=\nabla^{-2}f\left(\boldsymbol{r}\right)-k^{-2}\epsilon e^{i\boldsymbol{k}.r}$$

  - So the inverse operator damps out the noise
- A key step in applying MADNESS to any problem is rewriting differential equations in integral form

Advantages of Integral Form

- E.g., $\nabla^2 u(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r})$ v.s. $u(r) = \int G(\boldsymbol{r}, \boldsymbol{r}')\rho(\boldsymbol{r}')d^3r'$
  - Often soluble without any preconditioning and often without any iteration (as in this case)
  - Can obtain higher accuracy
  - In simple domains builds in correct asymptotics
  - Potentially more computationally efficient
- Challenge and solution
  - In most bases integral operator is dense & slow
  - Multiresolution analysis provides fast algorithms with guaranteed precision

Electrostatics $\nabla^2 u(\boldsymbol{r}) = -4\pi\rho(\boldsymbol{r})$

$$\begin{aligned} u(r) &= \int G(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d^3r' + \\ &\oint_{\partial\Omega}\left[G(\boldsymbol{r},\boldsymbol{r}')\boldsymbol{\nabla}'u(\boldsymbol{r}') - u(\boldsymbol{r}')\nabla' G(\boldsymbol{r},\boldsymbol{r}')\right].\boldsymbol{dS} \\ G(\boldsymbol{r},\boldsymbol{r}') &= \frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} \end{aligned}$$

Quantum mechanics $\left(-\frac{1}{2}\nabla^2 + V(\boldsymbol{r})\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$

$$\psi(\boldsymbol{r}) = -2\left(\nabla^2 + 2E\right)^{-1}V(\boldsymbol{r})\psi(\boldsymbol{r})$$

Time evolution $\hat{L}u(\boldsymbol{r},t) + N(u,t) = \frac{du}{dt}$

$$u(\boldsymbol{r},t) = e^{t\hat{L}}u(\boldsymbol{r},0) + \int_0^t e^{(\tau-t)\hat{L}}N(u,\tau)d\tau$$

$$e^{t\nabla^2}f(\boldsymbol{r}) = (4\pi t)^{-d/2}\int e^{-\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{4t}}f(r')d^d r$$

Integral Operator Formulation

- Solving the integral equation
  - Eliminates the derivative operator and related "issues"
  - Converges as fixed point iteration *with no preconditioner*

$$\left(-\tfrac{1}{2}\nabla^2 + V\right)\Psi = E\Psi$$

$$\Psi = -2\left(-\nabla^2 - 2E\right)^{-1} V\Psi$$

$$= -2G * \left(V\Psi\right)$$

$$\left(G * f\right)(r) = \int ds \frac{e^{-k|r-s|}}{4\pi|r-s|} f(s) \text{ in 3D ; } k^2 = -2E$$

Such Green's Functions (bound state Helmholtz, Poisson) can be rapidly and accurately applied with a single, sparse matrix vector product.

Separated form for integral operators

$$T * f = \int ds\, K(r-s) f(s)$$

- Approach
  - Represent the kernel over a finite range as a sum of products of 1-D operators (often, not always, Gaussian)

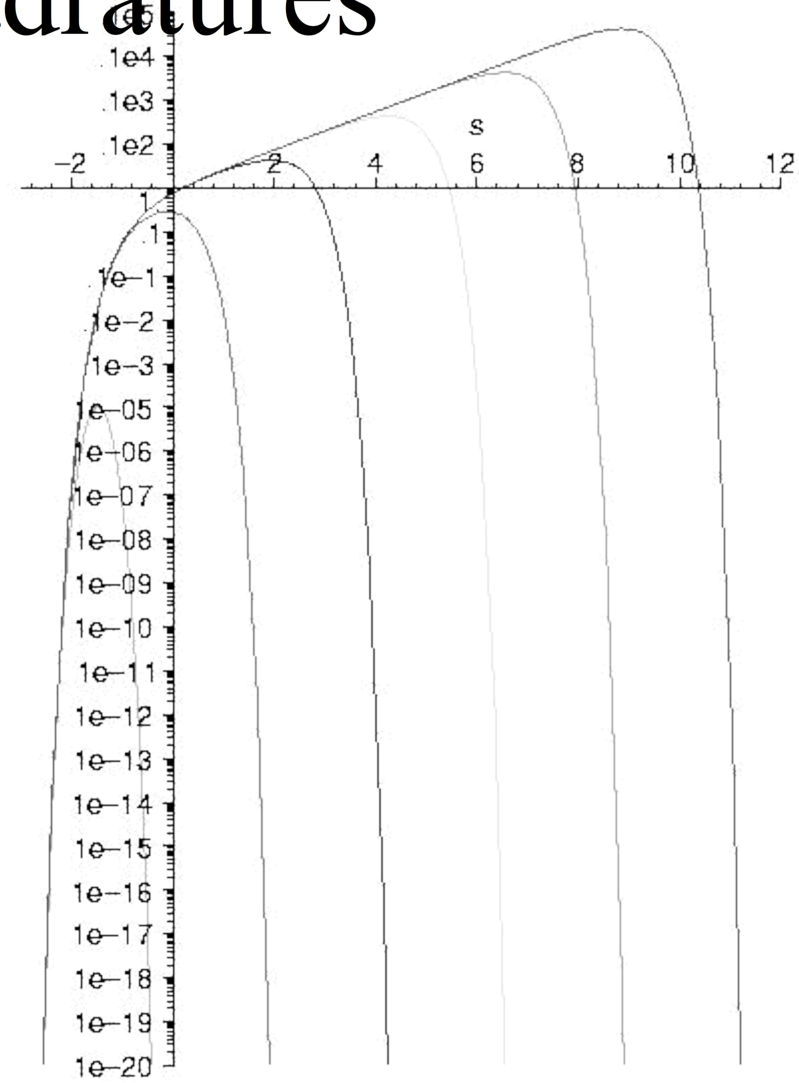
$$r_{ii',jj',kk'}^{n,l-l'} = \sum_{\mu=0}^{M} X_{ii'}^{n,l_x-l'_x} Y_{jj'}^{n,l_y-l'_y} Z_{kk'}^{n,l_z-l'_z} + O(\epsilon)$$

  - Only need compute 1D transition matrices (X,Y,Z)
  - SVD the 1-D operators (low rank away from singularity)
  - Apply most efficient choice of low/full rank 1-D operator
  - Even better algorithms slowly being implemented

Accurate Quadratures

$$
\begin{aligned}
\frac{e^{-\mu r}}{r} &= \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-x^2 t^2 - \mu^2/4t^2}\, dt \\
&= \frac{2}{\sqrt{\pi}} \int_{-\infty}^\infty e^{-x^2 e^{2s} - \mu^2 e^{-2s}/4 + s}\, ds \\
&= \sum_\mu c_\mu e^{t_\mu x^2} + O(\epsilon(m))
\end{aligned}
$$

- Trapezoidal quadrature
  - Geometric precision for periodic functions with sufficient smoothness
- Beylkin & Monzon
  - Further reductions



The kernel for x=1e-4,1e-3,1e-2,1e-,1e0.

The curve for x=1e-4 is the rightmost

Do new science with

O(1) programmers
O(100,000) nodes
O(100,000,000) cores
O(1,000,000,000) threads & growing

- Increasing intrinsic complexity of science
- Complexity kills … sequential or parallel
  - Expressing concurrency at extreme scale
  - Managing the memory hierarchy
- Semantic gap (Colella)
  - Why are equations O(100) lines but program is O(1M)
  - What's in the semantic gap – and how to shrink it?

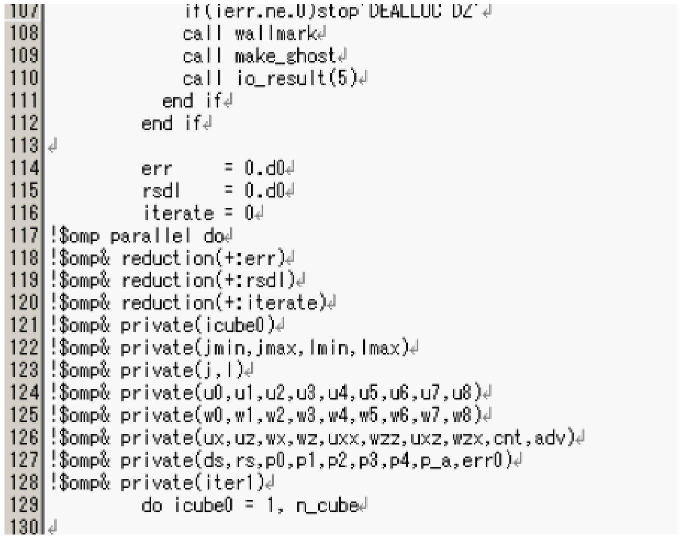
Wish list

- Eliminate gulf between theoretical innovation in small groups and realization on high-end computers
- Eliminate the semantic gap so that efficient parallel code is no harder than doing the math
- Enable performance-portable “code” that can be automatically migrated to future architectures
- Reduce cost at all points in the life cycle

- Much of this is pipe dream – but what can we aspire to?

Scientific vs. WWW or mobile software

- Why are we not experiencing similar exponential growth in functionality?
  - Level of investment; no. of developers?
  - Lack of software interoperability and standards?
  - Competition not cooperation between groups?
  - Shifting scientific objectives?
  - Are our problems intrinsically harder?
  - Failure to embrace/develop higher levels of composition?
  - Different hardware complexity?



```
                if(ierr.ne.0)stop'DEALLOC DZ'
                call wallmark
                call make_ghost
                call io_result(5)
              end if
            end if

            err      = 0.d0
            rsdl     = 0.d0
            iterate = 0
!$omp parallel do
!$omp& reduction(+:err)
!$omp& reduction(+:rsdl)
!$omp& reduction(+:iterate)
!$omp& private(icube0)
!$omp& private(jmin,jmax,lmin,lmax)
!$omp& private(j,l)
!$omp& private(u0,u1,u2,u3,u4,u5,u6,u7,u8)
!$omp& private(w0,w1,w2,w3,w4,w5,w6,w7,w8)
!$omp& private(ux,uz,wx,wz,uxx,wzz,uxz,wzx,cnt,adv)
!$omp& private(ds,rs,p0,p1,p2,p3,p4,p_a,err0)
!$omp& private(iter1)
            do icube0 = 1, n_cube

```

How do we write code for a machine that does not yet exist?

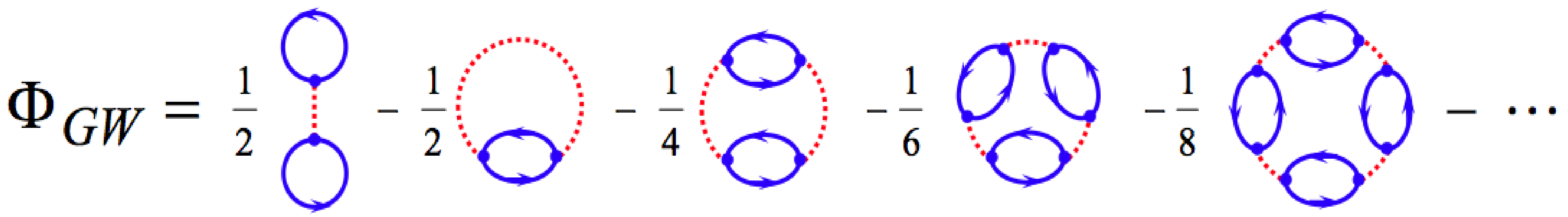
- Nothing too exotic, e.g., the mix of SIMD and scalar units, registers, massive multi-threading, software/hardware managed cache, fast/slow & local/remote memory that we expect in 2018+
- Answer 1: presently cannot
  - but it’s imperative that we learn how and deploy the necessary tools
- Answer 2: don’t even try!
  - where possible generate code from high level specs
  - provides tremendous agility and freedom to explore diverse architectures

Dead code

- Requires human labor
  - to migrate to future architectures, or
  - to exploit additional concurrency, or
  - ...
- By these criteria most extant code is dead
- Sanity check
  - How much effort is required to port to hybrid cpu+GPGPU?

7 December 1969

The language of many-body physics


$\Phi_{GW} = \frac{1}{2} \quad - \frac{1}{2} \quad - \frac{1}{4} \quad - \frac{1}{6} \quad - \frac{1}{8} \quad - \cdots$
Hartree
Fock
Infinite chain of ***dressed*** electron-hole bubbles

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]
```

$$\bar{h}_{ij}^{ab} = \left\langle \begin{matrix} a\,b \\ i\,j \end{matrix} \right| e^{-\hat{T}_1 - \hat{T}_2}\,\hat{H}\,e^{\hat{T}_1 + \hat{T}_2} \left| 0 \right\rangle$$

The Tensor Contraction Engine: A Tool for Quantum Chemistry

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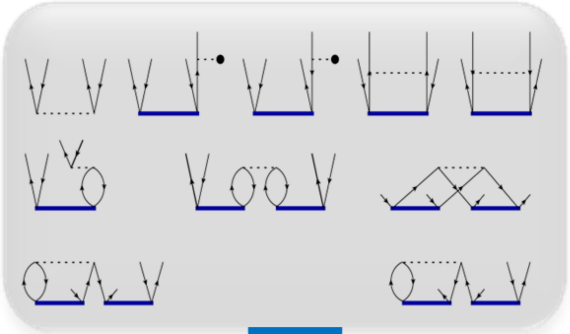
Tensor Contraction Engine (TCE) (Kowalski, PNNL)

Highly parallel codes are needed in order to apply the CC theories to larger molecular systems

Symbolic algebra systems for coding complicated tensor expressions: Tensor Contraction Engine (TCE)

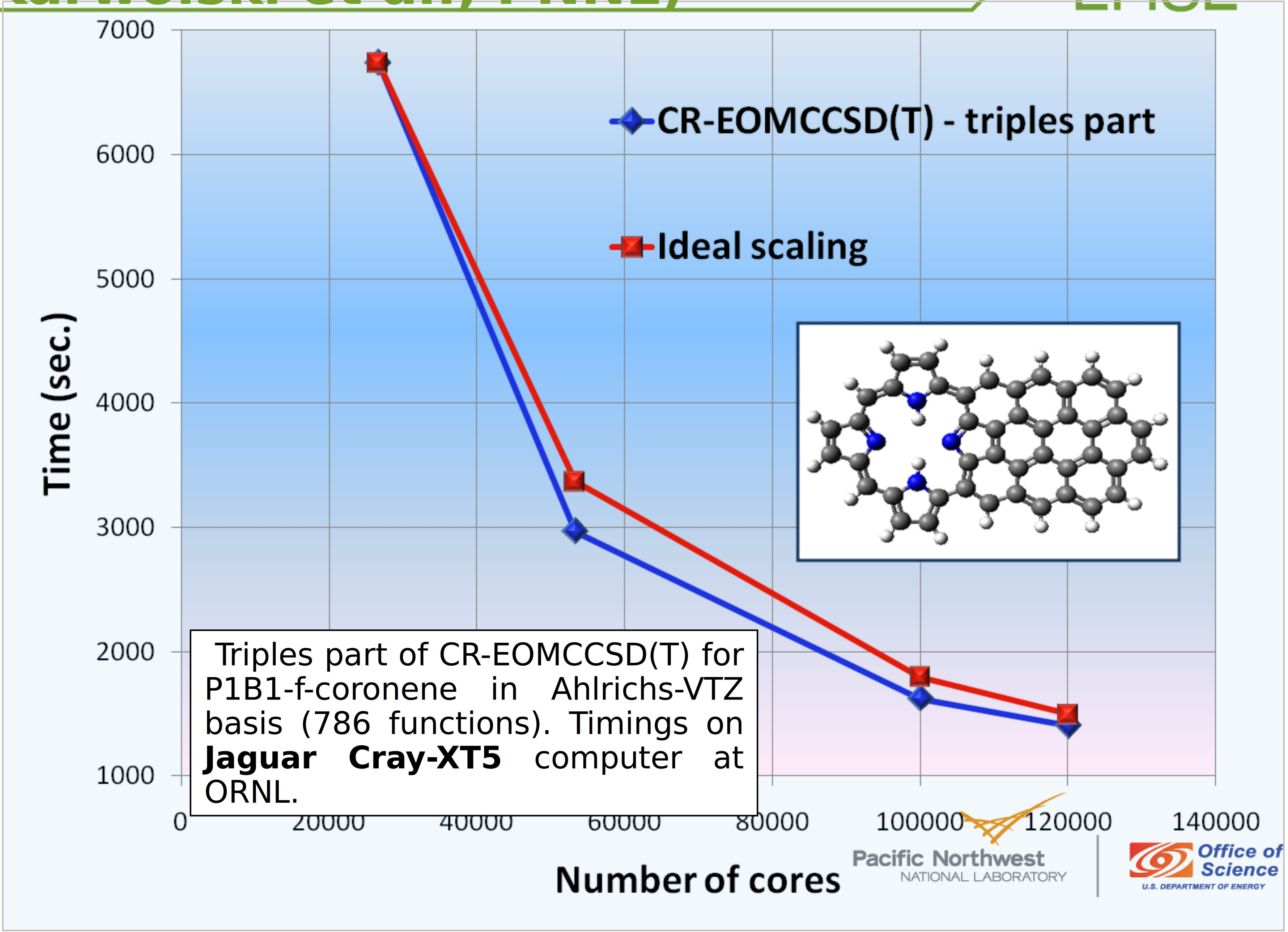
		Expression[a]
$D_i^a t_i^a$	=	$f_i^a + t_i^f I_f^a - t_n^a I_i^{\prime n} + t_{ni}^{fa} I_f^n + t_n^f v_{fi}^{na} - \frac{1}{2} t_{no}^{fa} v_{fi}^{no} + \frac{1}{2} t_{ni}^{fg} v_{fg}^{na} + \frac{1}{4} t_{ino}^{afg} v_{fg}^{no}$
$D_{ij}^{ab} t_{ij}^{ab}$	=	$v_{ij}^{ab} + P(a/b) I_f^a t_{ij}^{fb} - P(i/j) I_i^n t_{nj}^{ab} + \frac{1}{2} t_{ij}^{fg} I_{fg}^{\prime ab} + \frac{1}{2} t_{no}^{ab} I_{ij}^{no}$ $+ P(a/b) P(i/j) t_{in}^{af} I_{fj}^{nb} \frac{1}{2} P(a/b) I_{fg}^{na} t_{nij}^{fgb}$ $- \frac{1}{2} P(i/j) I_{fi}^{no} t_{noj}^{fab} + t_{nij}^{fab} I_f^n + P(i/j) t_i^f I_{fj}^{\prime ab} - P(a/b) t_n^a I_{ij}^{\prime nb} + \frac{1}{4} t_{ijno}^{abfg} v_{fg}^{no}$
$D_{ijk}^{abc} t_{ijk}^{abc}$	=	$P(a/bc) I_f^a t_{ijk}^{fbc} - P(i/jk) I_i^n t_{njk}^{abc} + \frac{1}{2} P(a/bc) t_{ijk}^{afg} I_{fg}^{bc} + \frac{1}{2} P(i/jk) t_{ino}^{abc} I_{jk}^{no}$ $+ P(ab/c) P(ij/k) t_{ijn}^{abf} I_{fk}^{nc} + P(a/bc) P(ij/k) t_{ij}^{af} I_{fk}^{bc} - P(ab/c) P(i/jk) t_{in}^{ab} I_{jk}^{\prime\prime nc}$ $+ t_{nijk}^{fabc} I_f^n + \frac{1}{2} P(a/bc) I_{fg}^{na} t_{nijk}^{fgbc} - P(i/jk) I_{fi}^{no} t_{nojk}^{fabc} + \frac{1}{4} t_{ijkno}^{abcfg} v_{fg}^{no}$
$D_{ijkl}^{abcd} t_{ijkl}^{abcd}$	=	$P(a/bcd) I_f^a t_{ijkl}^{fbcd} - P(i/jkl) I_i^n t_{njkl}^{abcd} + \frac{1}{2} P(ab/cd) t_{ijkl}^{abfg} I_{fg}^{cd} + \frac{1}{2} P(ij/kl) t_{ijno}^{abcd} I_{kl}^{no}$ $+ P(abc/d) P(ijk/l) t_{ijkn}^{abcf} I_{fl}^{nd} + P(ab/cd) P(ijk/l) t_{ijk}^{abf} I_{fl}^{cd} - P(abc/d) P(ij/kl) t_{ijn}^{abc} I_{kl}^{nd}$ $+ P(a/bcd) P(ij/kl) t_{ij}^{af} I_{fkl}^{\prime bcd} - P(ab/cd) P(i/jkl) t_{in}^{ab} I_{jkl}^{\prime ncd} + P(ab/cd) P(ij/kl) t_{ijn}^{abf} I_{jk}^{\prime ncd}$ $+ \frac{1}{2} P(abc/d) P(i/jkl) t_{ino}^{abc} I_{jkl}^{\prime nod} + t_{nijkl}^{fabcd} I_f^n + \frac{1}{2} P(a/bcd) I_{fg}^{na} t_{nijkl}^{fgbcd}$ $- \frac{1}{2} P(i/jkl) I_{fi}^{no} t_{nojkl}^{fabcd}$
$D_{ijklm}^{abcde} t_{ijklm}^{abcde}$	=	$P(a/bcde) I_f^a t_{ijklm}^{fbcde} - P(i/jklm) I_i^n t_{njklm}^{abcde} + \frac{1}{2} P(abc/de) t_{ijklm}^{abcfg} I_{fg}^{de} + \frac{1}{2} P(ijk/lm) t_{ijkno}^{abcde} I_{lm}^{no}$ $+ P(abcd/e) P(ijkl/m) t_{ijkln}^{abcdf} I_{fm}^{ne} + P(abc/de) P(ijk/lm) t_{ijkn}^{abcf} I_{flm}^{\prime\prime nde}$ $+ \frac{1}{2} P(abcd/e) P(ij/klm) t_{ijno}^{abcd} I_{klm}^{\prime noe} + \frac{1}{2} P(ab/cde) P(ijkl/m) t_{ijkl}^{abfg} I_{fgm}^{\prime cde}$ $+ P(abc/de) P(ijkl/m) t_{ijkl}^{abcf} I_{fm}^{de} - P(abcd/e) P(ijk/lm) t_{ijkn}^{abcd} I_{lm}^{ne}$ $+ P(ab/cde) P(ijk/lm) t_{ijk}^{abf} I_{flm}^{\prime\prime cde} - P(abc/de) P(ij/klm) t_{ijn}^{abc} I_{klm}^{nde}$ $+ P(a/bcde) P(ij/klm) t_{ij}^{af} I_{fklm}^{\prime bcde} - P(ab/cde) P(i/jklm) t_{in}^{ab} I_{jklm}^{\prime ncde}$



$$+\frac{1}{4} v_{ef}^{mn} t_{ij}^{ef} t_{mn}^{ab} - \frac{1}{2} v_{ef}^{mn} t_{mi}^{ef} t_{nj}^{ab} +$$

```
next = NXTASK(nprocs, 1)
DO p3b = noab+1,noab+nvab
DO p4b = p3b,noab+nvab
DO h1b = 1,noab
DO h2b = h1b,noab
IF (next.eq.count) THEN
CALL GET_HASH_BLOCK(d_a,dbl_mb(k_a),dim
- 1 + (noab+nvab) * (h1b_1 - 1 + (noab+
+nvab) * (p3b_1 - 1)))))
CALL GET_HASH_BLOCK_I(d_a,dbl_mb(k_a),d
```

Parallel performance (Karwolski et al., PNNL)

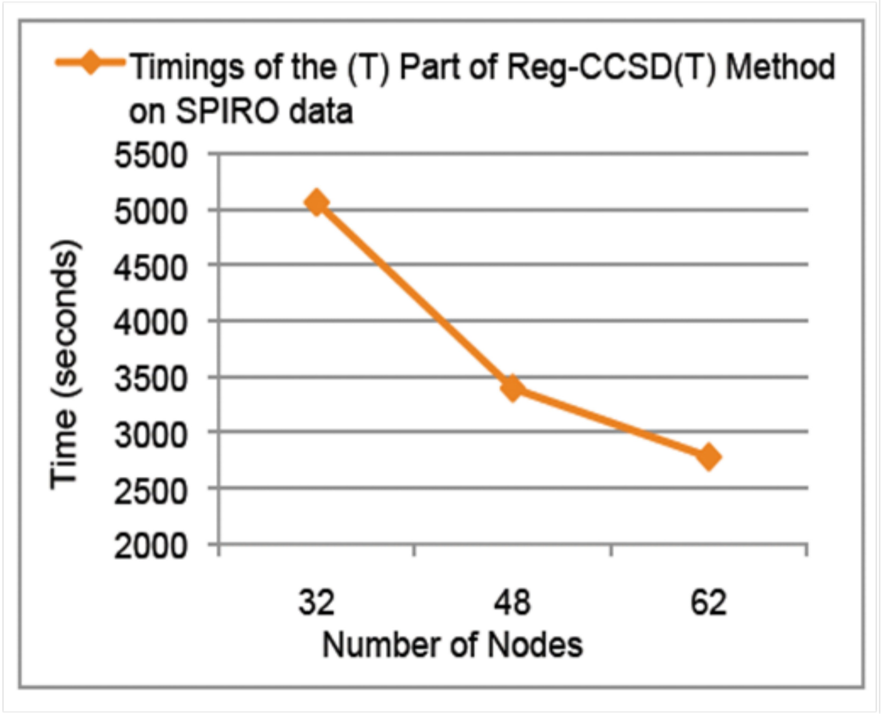


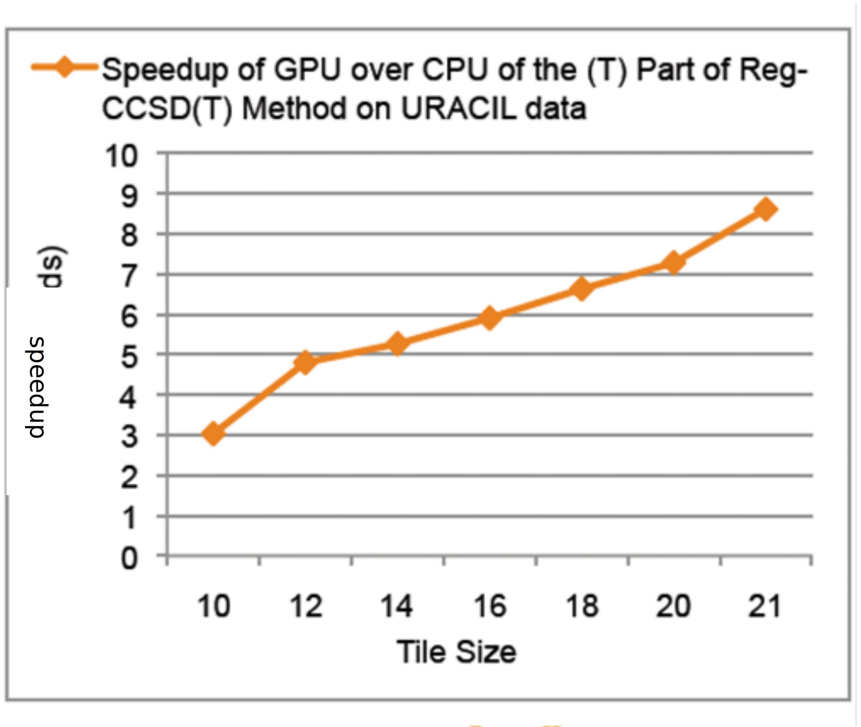
Triples part of CR-EOMCCSD(T) for P1B1-f-coronene in Ahlrichs-VTZ basis (786 functions). Timings on **Jaguar Cray-XT5** computer at ORNL.

Towards future computer architectures (Villa,Krishnamoorthy, Kowalski)

The CCSD(T)/Reg-CCSD(T) codes have been rewritten in order to take advantage of GPGPU accelerators

Preliminary tests show very good scalability of the most expensive N7 part of the CCSD(T) approach


Timings of the (T) Part of Reg-CCSD(T) Method on SPIRO data
Time (seconds)
Number of Nodes


Speedup of GPU over CPU of the (T) Part of Reg-CCSD(T) Method on URACIL data
speedup
Tile Size