Accelerated Cartesian Expansions (ACE): A Linear Scaling Method for the Rapid Evaluation of Pairwise Interactions

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Overview

Motivation

The numerical solution to many problems in applied physics involve the evaluation of spatial or spatio-temporal convolutions, i.e., potentials.

- Iterative solution of (boundary) integral equations
- Marching-on-in-time (MOT) methods for time domain integral equations
- Computation of forces and energies in molecular/particle dynamics
- Evaluation of the Hartree/Fock fields in electronic structure calculations

- Cost of evaluating spatial potentials: $\mathcal{O}(N_s^2)$
- Cost of evaluating spatio-temporal potentials: $\mathcal{O}(N_s^2 N_t^2)$
- With ACE, these are reduced to $\mathcal{O}(N_s)$ and $\mathcal{O}(N_s N_t \log^2(N_t))$

Problem Statement

- We consider some open domain, $\Omega \subset \mathbb{R}^D$, in which some 'source' function, $\rho(\vec{\mathbf{r}})$ is supported.
- $\rho(\vec{\mathbf{r}})$ gives rise to some potential, $\phi(\vec{\mathbf{r}})$, that obeys the following equation:

$$\mathcal{L}\phi(\vec{\mathbf{r}}) = \rho(\vec{\mathbf{r}}),\ \vec{\mathbf{r}} \in \Omega \qquad \mathcal{T}\phi(\vec{\mathbf{r}}) = b(\vec{\mathbf{r}}),\ \vec{\mathbf{r}} \in \partial\Omega \tag{1}$$

- $\mathcal{L}$ is a linear operator, the inverse of which is associated with some Green's function, $G(\vec{\mathbf{r}}, \vec{\mathbf{r}}')$, uniquely determined defined by boundary conditions embodied by $\mathcal{T}$.
- The resolution of $\phi(\vec{\mathbf{r}})$ can be reduced to convolution(s) of the form:

$$\phi(\vec{\mathbf{r}}) = \int d^D\vec{\mathbf{r}}' G(\vec{\mathbf{r}}, \vec{\mathbf{r}}') f(\vec{\mathbf{r}}') \rightarrow \mathbf{\Phi} = \mathbf{GP} \tag{2}$$

- Sampling/calculating $\rho(\vec{\mathbf{r}})$ and $\phi(\vec{\mathbf{r}})$ at N points $\rightarrow \mathbf{\Phi}$ and $\mathbf{P}$
- Convolution = matrix-vector multiplication $\rightarrow \mathcal{O}(N^2)$ cost
- The ACE algorithm reduces this cost to $\mathcal{O}(N)$

ACE Algorithm

History and Features

ACE is a hierarchical, tree-based method, similar in spirit to the Fast Multipole Method (FMM) of Greengard and Rokhlin. It has been applied to the solution of numerous problems:

- Evaluation of pairwise potentials with long-range interactions, i.e., $V(||\vec{\mathbf{r}} - \vec{\mathbf{r}}'||) = ||\vec{\mathbf{r}} - \vec{\mathbf{r}}'||^{-\nu}, \forall \nu \in \mathbb{R}$
- Wideband, multiscale EM/optics problems in free space.
- Electrically dense periodic EM/optics problems.
- Time domain problems with diffusive/dissipative tails (diffusion, lossy wave, and Klein-Gordon potentials)
- Lienard-Wiechert and time domain Floquet potentials
- Generalized periodic problems, including Yukawa and Coulomb fields

Some of the salient features of ACE include:

- Totally linear cost in terms of memory and FLOPs
- Amenability to non-uniform discretization
- Exact up/down tree traversal
- Nearly kernel independent

Algorithmic Details

The ACE algorithm maps the matrix-vector product in Eqn. (2) onto:

$$\mathbf{GP} = \mathbf{G}_{\mathbf{near}}\mathbf{P} + \mathcal{A}_{ACE}(\mathbf{P}) \tag{3}$$

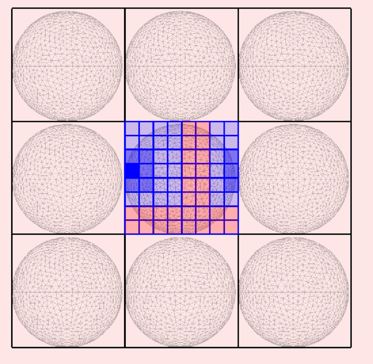
$\mathbf{G}_{\mathbf{near}}$ is a sparse matrix with $\mathcal{O}(N)$ entries that describes 'near' interactions, and $\mathcal{A}_{ACE}$ is a composition of operators that effects the remaining 'far' interactions.

The ACE algorithm essentially reduces to two components:

- A means of distinguishing between 'near' and 'far' interactions
- Addition theorems that formalize the manner in which 'far' interactions are effected in $\mathcal{O}(N)$ time $\rightarrow$ tree traversal

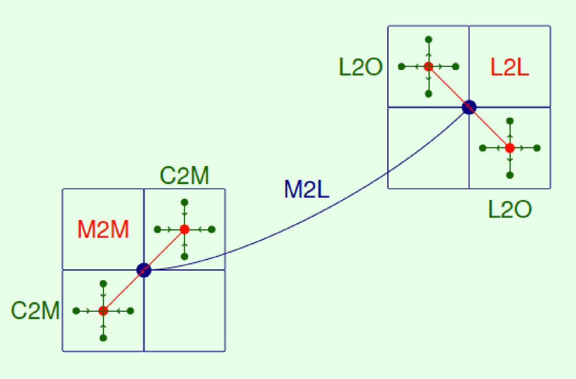
This is facilitated by constructing an octree decomposition of Ω

- Ω is embedded inside a cubic domain and recursively divided into smaller cubic boxes until desired level of refinement is achieved.
- (Right) 4 level octree decomposition of Ω for a periodic problem. Interaction list for the dark blue box is color-coded.



- Blue boxes are in the nearfield, light blue boxes are in the farfield, and red boxes are accounted for at a higher level of the tree.

- Tree traversal effects the farfield contribution to the total potential by the construction of a hierarchical expansion in Cartesian harmonics.



- **C2M:** Point sources aggregated to create multipole tensors, $\mathbf{M}^{(n)}$
- **M2M:** Multipole origins shifted/aggregated
- **M2L:** Multipole expansion translated to local expansion, $\mathbf{L}^{(n)}$
- **L2L:** Local origins shifted/disaggregated
- **L2O:** Local tensors mapped onto potential at point observers

- Multipole to local translation maps onto Taylor Expansion for the Green's function truncated at Pth order:

$$\mathbf{L}^{(n)} = \sum_{m=n}^{P} \frac{1}{n!}\mathbf{M}^{(m-n)} \cdot (m-n) \cdot \nabla^{(n)} G(|\vec{\mathbf{r}}_o^p - \vec{\mathbf{r}}_s^p|) \tag{4}$$

- Formulation in terms of totally symmetric Cartesian tensors bolsters efficiency relative to conventional Taylor-based methods.

Results

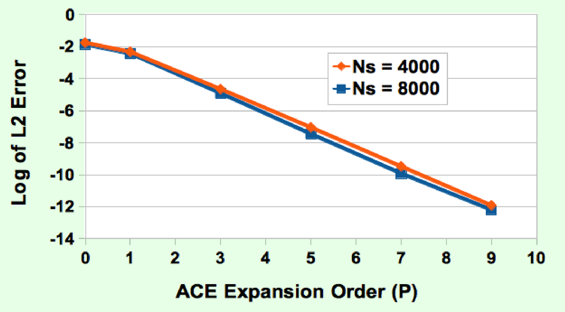
Error Convergence

- Error in the ACE expansion was calculated for $G(|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|) = |\vec{\mathbf{r}} - \vec{\mathbf{r}}'|^{-2.2}$ for trees of varying height, N_l, and different ACE expansion orders, P .

P	$N_l = 3$	$N_l = 5$	$N_l = 7$	$N_l = 10$
2	$3.268070962493116E-003$	$3.268070962493099E-003$	$3.268070962493107E-003$	$3.268070962493042E-003$
5	$2.866109269813751E-005$	$2.866109269813507E-005$	$2.866109269812455E-005$	$2.866109269808440E-005$
8	$4.207517301400774E-007$	$4.207517302158528E-007$	$4.207517301963213E-007$	$4.207517301868480E-007$
11	$7.470454043399749E-009$	$7.470454038637677E-009$	$7.470454030684618E-009$	$7.470454009643825E-009$

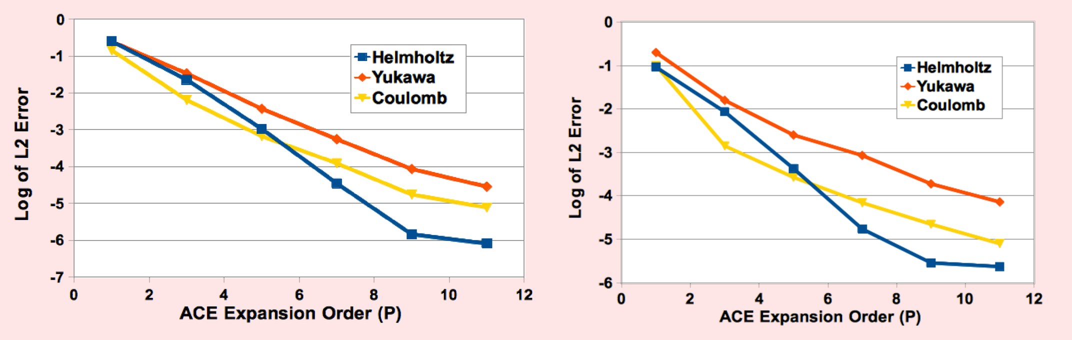
- Error decreases rapidly in P, independent of the height of the tree.
- This is a demonstration of the exact up/down tree traversal operators specific to ACE.

- Relative ACE error for a spatio-temporal potential (diffusion) was evaluated and compared to an exact result.



- Relative error decreases very rapidly with the order of the ACE expansion. 12 digits are retained for a 9th order expansion.

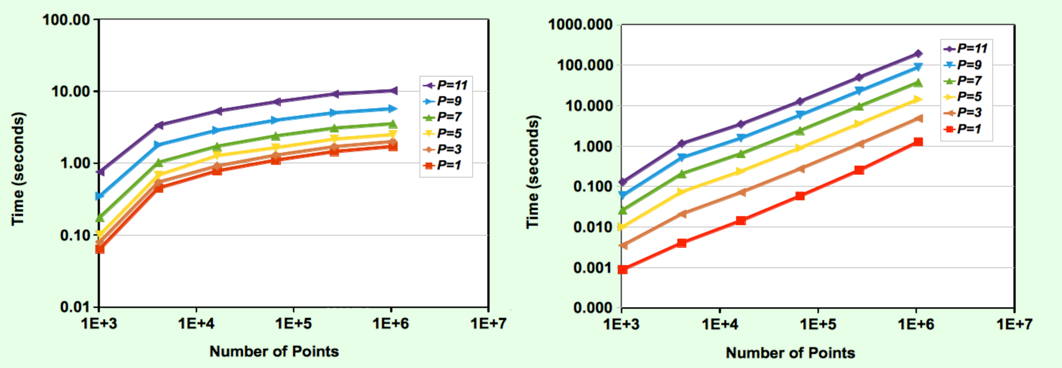
- Relative ACE error for periodic long-range potentials were evaluated and compared to an exact results.



- Error for doubly periodic (left) and triply periodic (right) systems all converge rapidly in P, nearly independent of potential.
- Presently, Dan Dault is implementing time domain periodic ACE.

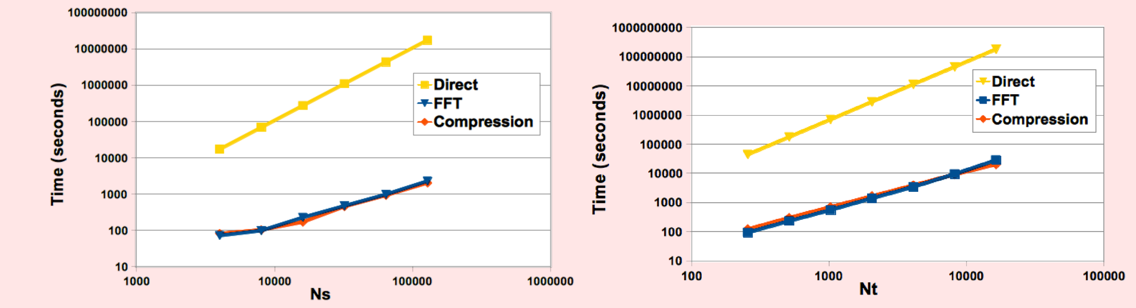
Scaling

- The doubly periodic Helmholtz potential was evaluated using ACE, timings were measured to illustrate scaling in the frequency domain.



- Scaling of precomputation (left) / tree traversal (right) with varying P.
- Precomputation scales sublinearly in the number of levels, tree traversal scales as $\mathcal{O}(N_s^{1.03})$ in the worst case.

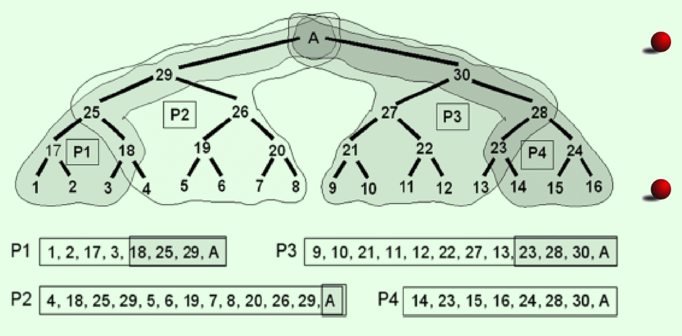
- Spatio-temporal potentials accelerated using ACE in space, and 1 of 2 temporal schemes: FFTs or recursive block-Toeplitz compression.



- Scaling in space (left) / time (right) for both FFT- and compression-based schemes, compared to direct convolution.
- Considerable savings: $\mathcal{O}(N_s^2 N_t^2) \rightarrow \mathcal{O}(N_s N_t \log^2(N_t))$

Parallelism

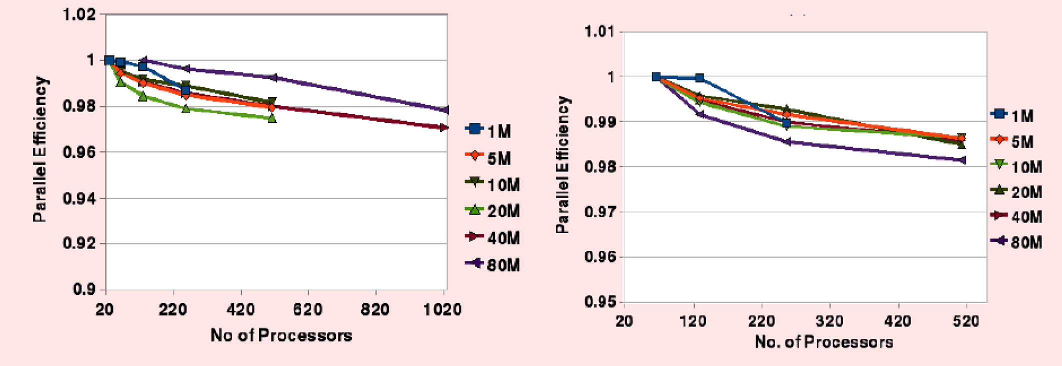
- Tree-based methods are manifestly difficult to parallelize.
- Our MPI implementation of ACE has high parallel efficiency due to a parallel algorithm designed by alumnus, Melapudi Vikram.



- Points Distributed across processors based upon spatial partitioning.
- Local tree built on each processor, filling entire computational domain.

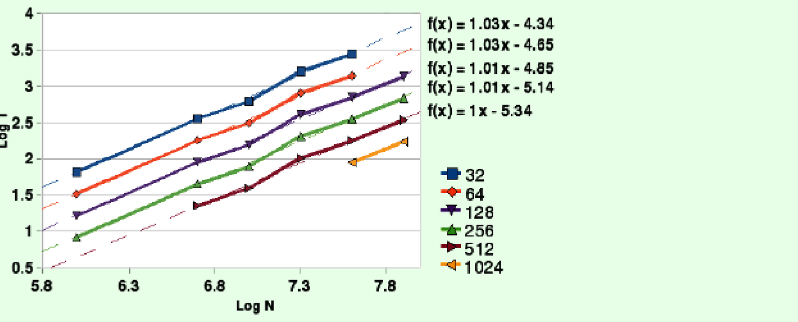
- Nodes appear in more than one processor $\rightarrow$ post-order traversal of local tree $\rightarrow$ natural means of assigning a native processor.
- Redundancy all the way up the tree leads to implicit load balancing.

- Parallel efficiency of tree traversal was measured for two different point distributions - a cubical volume (left), and a spherical surface (right) - for a composite Lennard-Jones/Coulomb force field.



- Different lines correspond to different problem sizes.
- Parallel efficiency of $96\%+$ for up to 1024 processors and 80 million particles.

- Total runtime for a single force/potential evaluation was measured as the number of particles and number of processors are varied.



- Regression indicates linear scaling in all cases - $N^{1.03}$ scaling at worst.

Conclusions

The ACE algorithm is a flexible and efficient framework for the evaluation of spatial and temporal convolutions that arise in the solution of numerous partial differential equations and integral equations. To this end, we have demonstrated:

- Convergence to arbitrary error with expansions of increasing order
- Linear scaling evaluation of pairwise potentials, and accelerated spatio-temporal potentials.
- Parallel efficiency for very large problems.

Acknowledgements

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