Projector Augmented Wave-based Kohn-Sham Density Functional Theory in *OpenAtom* with $N^2 \log N$ scaling

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Goal: The study of complex heterogeneous systems to discern emergent and new physics and create impact.

Approach:

Scientific Insight
From Modeling
Software

Methods

Physics-based solutions for complex systems
**OpenAtom Concept:** Statistical Sampling of Complex Environments is Key to Understanding many Physical Systems.

**Biological function**: enabled by fluctuations in both the environment and the biomolecules.

**Pollutant detection**: requires sampling complex aqueous systems and then exporting the results to a GW/GW-BSE app for computation of spectra.

**Understanding chemical reactions in dense arrays**: requires non-trivial sampling of the full system due to complex many-body reaction paths.

**OpenAtom**: Pimpernel (Martyna), UIUC (Kale) and Yale (Ismail-Beigi) collaborate to build the Electronic Ground and Excited State parallel software and methods including classical and quantum nuclear motion capabilities to realize this vision.
Key Project Accomplishments thus Far:

Electronic Ground State (charm++ parallelization):
1. High Parallel Scaling allows study of hydrogen storage in MOF’s via Path Integral CPAIMD.
2. Exact Exchange $N^2 N^{1/3} \log N$ (for metals & insulators): 10x speed 32 waters! (SIAM in prep).
3. Projector Augmented Wave method in $N^2 \log N$ (new results!).

Electronic Excited States (charm++ parallelization)
1. High Parallel Scaling for $O(N^4)$ GW
2. $O(N^3)$ GW method based on a shredded propagator, complex time formalism

Reduced order GW software soon to be released!

- **KS-DFT:** *Ground state electronic energy* expressed *exactly* as the *minimum of a functional of the zero temperature, 1-body density* written in terms of

\[
\rho(r, r') = \sum_{i=1}^{N_{KS}} \psi_i(r)\psi_i^*(r'), \quad n(r) = \rho(r, r), \quad N_{KS} = (# \text{ electrons})/2
\]

an orthonormal set of KS states, \(< \psi_i \mid \psi_j > = 2\delta_{ij} >.

- **KS Density Functional:** *Sum of the kinetic energy* of non-interacting electrons, *Hartree energy, electron-ion/external energy* and an unknown correction term, *exchange correlation energy functional*,

\[
E[n(r)] = -\frac{\hbar^2}{2m_e} \int dr \left( \nabla^2 \rho(r, r') \right)|_{r'=r} + \frac{e^2}{2} \int dr dr' \frac{n(r)n(r')}{|r - r'|} + e \int dr n(r)V_{\text{ext}}(r; N) + E_{xc}[n(r)], \quad N = # \text{ ions, } N_{KS} \sim N.
\]

- **Generalized Gradient Approximation (GGA):** *Tractable approx. to* \(E_{xc} \)

\[
E_{xc}[n(r)] \approx \int dr \, \varepsilon_{xc}(n(r), \nabla n(r))
\]
KS-DFT in OpenAtom

- **OpenAtom**: *Plane-wave* (PW) based KS-DFT within the GGA – expand KS states in the delocalized PW basis.

- **PW-KS-DFT in OpenAtom - Advantages:**
  - $N^2 \log N$ or better scaling of interactions & derivatives - *Euler Exponential Spline (EES) Interpolation*.
  - Only orthogonalization is $\sim N^3$.
  - *High parallelism under charm++*.
  - k-points, path integrals, LSDA & tempering implemented.

- **PW-KS-DFT in OpenAtom - Disadvantages:**
  - *Large basis set* required - millions and millions (c.f. Carl Sagan).
  - *Large memory* required – need large machines.
  - *Heavy atoms (impossibly) computationally intensive*. 
Projector Augmented Wave Method (PAW)


• Projector-Augmented Wave (PAW) : accurate treatment of heavy atoms in KS-DFT with low computational cost.

• PAW-KS-DFT Advantages
  o KS states split into localized and delocalized/smooth parts – small basis possible even for heavy atoms.
  o NMR and some other linear response methods require the core – PAW makes it easy.
  o Small memory requirement.

• PAW-KS-DFT Disadvantages
  o Implemented with inefficient $N^3$ methods for interactions.
  o Parallel performance of standard implementations poor.
  o Accuracy control poor.

Goal: Implement $N^2 \text{log} N$ EES-based PAW with high parallel efficiency in OpenAtom.
**PAW Basics: KS states**

- **KS states:** *delocalized/smooth part, (S), + localized/core part, (core).*
  
  Core localized within a sphere of radius $R_{pc}$ around each ion:
  
  $$\psi_I(r) = \psi_I^{(S)}(r) + \sum_{j=1}^{N} \psi_I^{(core)}(r), \quad \psi_I^{(core)}(r) = 0, |r - R_j| > R_{pc}$$

- **Smooth:** fills all spaces & varies, *expanded in plane-waves*:
  
  $$\psi_I^{(S)}(s) = \frac{1}{\sqrt{V}} \sum_{|g| \leq G_c/2} \tilde{\psi}_I^{(S)}(g) \exp(i\hat{g} s)$$
  
  $$r = hs, \quad V = \text{det} \ h, \quad g = 2\pi h^{-1} \hat{g}, \quad \hat{g} \in \text{integer}$$

- **Core:** localized, written in *terms of fixed core projectors, \{\Delta p, p^{(S)}\}*:  
  
  $$\psi_I^{(core)}(r) = \Delta p(r - R_j)Z_{ij}^{(S)}, \quad \Delta p(r - R_j) = 0, |r - R_j| > R_{pc}$$
  
  $$Z_{ij}^{(S)} = < p_j^{(S)}|\psi_i^{(S)}> = \int dr^3 p^{(S)}(r - R_j)\psi_i^{(S)}(r), \quad p^{(S)}(r - R_j) = 0, |r - R_j| > R_{pc}$$

* 1 ion type, 1 channel for simplicity
PAW Basics: Example KS state

\[
h = \begin{bmatrix} L_x & 0 & 0 \\ 0 & L_y & 0 \\ 0 & 0 & L_z \end{bmatrix}
\]

Localized ion core states, \( \psi_{IJ}^{(\text{core})}(r) \) embedded

in the smooth part of the state, \( \psi_I^{(S)}(r) \), that fills \( D(h) \).
PAW Basics: KS-DFT within LDA under periodic boundary conditions at $\Gamma$

The whole enchilada:

\[
E[n(r)] = E_{NIKE} + E_{ext} + E_H + E_{xc}
\]

\[
E_{NIKE} = -\frac{\hbar^2}{2m_e} \int_{D(h)} dr \sum_l \langle \psi_l | \nabla^2 | \psi_1 \rangle
\]

\[
E_{xc} = \int_{D(h)} dr \, \varepsilon_{xc}(n(r))
\]

\[
E_H = \frac{e^2}{2} \int_{D(h)} dr \int_{D(h)} dr' \sum_m \frac{n(r)n(r')}{|r - r' + mh|}
\]

\[
E_{ext} = -\int_{D(h)} dr \sum_j \sum_m \frac{eQ_j n(r)}{|r - r_j + mh|}
\]

Non-interacting electron kinetic energy: Smooth and core terms

\[
E_{NIKE} = E_{NIKE}^{(S)} + E_{NIKE}^{(core1)} + E_{NIKE}^{(core2)}
\]

\[
E_{NIKE}^{(S)} = -\frac{\hbar^2}{2m_e} \int_{D(h)} dr \sum_l \langle \psi_l^{(S)} | \nabla^2 | \psi_l^{(S)} \rangle,
E_{NIKE}^{(core1)} = -\frac{\hbar^2}{2m_e} \sum_{lj} Z_{lj}^{(S)} Z_{lj}^{(\nabla^2 \Delta)}\),
E_{NIKE}^{(core2)} = -\frac{\hbar^2}{2m_e} \sum_j Z_{j}^{(S,2)} \langle \Delta p | \nabla^2 | \Delta p \rangle
\]

Exchange Correlation energy: Smooth and core terms

\[
E_{xc} = E_{xc}^{(S)} + E_{xc}^{(core)} = \int_{D(h)} dr \, \varepsilon_{xc}(n^{(S)}(r)) + \sum_{j} \int_{D(R_{pc})} dr \left[ \varepsilon_{xc}(n_j(r)) - \varepsilon_{xc}(n_j^{(S)}(r)) \right]
\]

\[
n^{(S)}(r) = \sum_l |\psi_l^{(S)}(r)|^2,
\]

\[
n_j(r) = n^{(S)}(r - R_j) + n^{(core1)}(r - R_j) + n^{(core2)}(r - R_j),
n_j^{(S)}(r) = n^{(S)}(r - R_j)
\]

\[
\forall \ r \in D(h) \quad \forall |r - R_j| < R_{pc} \quad \forall |r - R_j| < R_{pc}
\]
PAW Basics: KS-DFT long/short-range decomposition

Due to the mixed localized and delocalized basis, there is no natural truncation scale for the long-range interactions of \( E_H \) and \( E_{\text{ext}} \) in \( \mathbf{g} \)-space or \( \mathbf{r} \)-space alone.

\[
E_H = \frac{e^2}{2} \int_{D(h)} \int_{D(h)} dr \, dr' \sum_m \frac{n(r)n(r')}{|r-r'+m\mathbf{h}|}, \quad E_{\text{ext}} = -\int_{D(h)} dr \, n(r) \sum_j \sum_m \frac{eQ_j}{|r-R_j+m\mathbf{h}|}
\]

Using Poisson summation and Ewald's decomposition of \( 1/r \):

\[
E_H = E_H^{(\text{short})} + E_H^{(\text{long})} \quad E_{\text{ext}} = E_{\text{ext}}^{(\text{short})} + E_{\text{ext}}^{(\text{long})}
\]

\[
E_H^{(\text{short})} = \frac{e^2}{2} \int_{D(h)} \int_{D(h)} dr \, dr' \frac{n(r)n(r')\text{erfc}(\alpha|r-r'|)}{|r-r'|} \quad E_{\text{ext}}^{(\text{short})} = -e \int_{D(h)} dr \, n(r) \sum_j \text{erfc}(\alpha|\mathbf{r-R}_j|) \frac{1}{|\mathbf{r-R}_j|}
\]

\[
E_H^{(\text{long})} = \frac{e^2}{2V} \sum_{g \neq 0} \frac{4\pi}{|\mathbf{g}|^2} \exp\left(-\frac{|\mathbf{g}|^2}{4\alpha^2}\right) |\bar{n}(\mathbf{g})|^2 - \frac{\pi e^2 |\bar{n}(0)|^2}{2V\alpha^2} \quad E_{\text{ext}}^{(\text{long})} = -\frac{e}{V} \sum_{g \neq 0} \frac{4\pi}{|\mathbf{g}|^2} \exp\left(-\frac{|\mathbf{g}|^2}{4\alpha^2}\right) \bar{n}(\mathbf{g})\bar{S}(\mathbf{g}) + \frac{\pi e\bar{n}(0)\bar{S}(0)}{V \alpha^2}
\]

\[
\bar{S}(\mathbf{g}) = \sum_j Q_j \exp(-i\mathbf{g} \cdot \mathbf{R}_j)
\]

Choose \( \alpha \), such that the \( \mathbf{g} \)-space cutoff = \( G_c \) = pw density cutoff.

Ensure \( \mathbf{r} \)-space cutoff, \( R_c = (3.5 / \alpha) > R_{pc} \), confines the \( m \)-sum to the 1st image.

Decompose short-range into smooth, core1 and core2 type terms, (not shown).
Accuracy of long/short decomposition

To approximately match long/short range accuracy: \( \frac{G_c^2}{4} \approx \frac{\gamma^4}{R_c^2} \), \( \gamma = \alpha R_c \)

<table>
<thead>
<tr>
<th>( R_c = 4 \text{ bohr} )</th>
<th>( \gamma = \alpha R_c )</th>
<th>( \text{erfc}(\gamma) )</th>
</tr>
</thead>
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<tr>
<td>PW cutoff: ( \frac{\hbar^2 G_c^2}{2\text{me}} ) Ryd</td>
<td>5.1</td>
<td>3.0</td>
</tr>
<tr>
<td></td>
<td>9.4</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>16</td>
<td>4.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( R_c = 2 \text{ bohr} )</th>
<th>( \gamma = \alpha R_c )</th>
<th>( \text{erfc}(\gamma) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PW cutoff: ( \frac{\hbar^2 G_c^2}{2\text{me}} ) Ryd</td>
<td>20.3</td>
<td>3.0</td>
</tr>
<tr>
<td></td>
<td>37.5</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>64</td>
<td>4.0</td>
</tr>
</tbody>
</table>

High accuracy can be obtained with both \( R_c \) and \( G_c \) small!
PAW Basics: Multi-Resolution, Grids, EES and $N^2 \log N$ scaling

How do we reduce scaling by one order in $N$ and maintain accuracy?

1. Discrete real-space: Fourier Coefficients and FFTs

- Given a discrete, $\mathbf{g} = 2\pi \mathbf{h}^{-1} \hat{\mathbf{g}}$, finite g-space, $|g| < G_c$, the Fourier coefficients, $\tilde{f}(\mathbf{g})$ of $f(\mathbf{r})$, can be converted to $\tilde{f}^m(\mathbf{g})$ from $f^m(\mathbf{r})$ exactly using an equally spaced s-space grid, $\mathbf{r} = \mathbf{h}s$, of side $N_{\text{FFT},\beta} > 2m\hat{g}_{\text{max}},_\beta \Delta s_{\beta} = 1/N_{\text{FFT},\beta}$. $\forall m \in \mathbb{Z} > 0$

- Using FFTs, the $\tilde{f}^m(\mathbf{g})$, can be computed exactly in $N \log N$ as:

$$f(s) = \frac{1}{V} \text{FFT}^\text{(m,+)}[\tilde{f}(\mathbf{g}), G_c], \quad \tilde{f}^m(\mathbf{g}) = \frac{V}{N_{\text{FFT}}} \text{FFT}^\text{(m,-)}[f^m(s), mG_c], \quad V = \det \mathbf{h}$$

2. Euler Exponential Spline Interpolation and FFTs

- To compute the $Z$-matrices, structure factors, $\tilde{S}(\mathbf{g})$, and core functions, fast, it is useful develop a differentiable controlled approximation to $\exp(i \mathbf{g} \cdot \mathbf{r})$ on a discrete $\mathbf{g}$-space for all $\mathbf{r} = \mathbf{h}s$ in $D(\mathbf{h})$ via interpolation from an equally spaced $s$-space grid, enabling the use of FFTs.

- The Euler exponential spline (EES) delivers where $M_p$ are the cardinal B-splines and $p$ the spline order,

$$e^{2\pi i \hat{\mathbf{g}} s} = D_p(\hat{\mathbf{g}}, N_{\text{FFT}}) \sum_{\hat{s} = 0}^{N_{\text{FFT}}} \sum_{j = 1}^p M_p(u - \hat{s}) e^{\frac{2\pi i \hat{\mathbf{g}} \hat{s}}{N_{\text{FFT}}}} \delta_{\hat{s},l-j} + O\left(\frac{2\hat{g}}{N_{\text{FFT}}}\right)^p, \quad M_p \text{ has compact supp.} \quad u = s N_{\text{FFT}} \quad l = \text{int } u \quad N_{\text{FFT}} > 2\hat{g}_{\text{max}} \approx 2.8\hat{g}_{\text{max}}$$

Using 3 FFT grids, (1) Psi EES, (2) Density, (3) Density EES, and 1 discrete spherical polar grid around each ion, $|\mathbf{r}| < R_{pc}$, all PAW energy terms & their derivatives can be accurately computed in $N^2 \log N$. 
PAW Basics: $g$-space to $s$-space and back

\[
\bar{\psi}^{(S,D)}_l (g) = \bar{\psi}^{(S)}_l (g) D^{(\psi)} (g)
\]

\[
F F T (\psi, +, E E S) \left[ \bar{\psi}^{(S,D)}_l (g), \frac{G}{2} \right]
\]

\[
\bar{\psi}^{(S)}_l (g) = \frac{V}{N_{F F T}^{(n,-)}} \left[ \bar{n}^{(S)} (s), G_c \right] 
\]

\[
\bar{n}^{(S,D)} (g) = \bar{n}^{(S)} (g) D^{(n)} (g)
\]

\[
F F T (n, +, E E S) \left[ \bar{n}^{(S,D)} (g), G_c \right]
\]

\[
\psi^{(S,D)}_l (s) = \frac{s}{N_{F F T}^{(\psi, E E S)}}
\]

\[
\left| \psi^{(S)}_l (s) \right|^2 = \frac{s}{N_{F F T}^{(\psi, E E S)}}
\]

\[
r = \h s
\]

The $D^{(\tau)} (g) = \prod_{\alpha} D_p \left( \hat{g}_\alpha, N_{F F T, \alpha}^{(\tau, E E S)} \right)$ enables B-spline interpolation.
PAW Basics: \( r \)-space interpolation

EES provides an accurate, differentiable interpolation between the different resolutions and length scales of PAW.

\begin{align*}
\text{Psi EES: } N^{(\psi,\text{EES})}_{\text{FFT}} & \sim N \\
\text{Density EES: } N^{(n,\text{EES})}_{\text{FFT}} & \sim N
\end{align*}

- \( h \) defines \( D(h) = \text{cuboid} \)
- \( V = \det h \sim N \)
- \( \psi_i^{(S,D)}(s) \)
- \( \text{FFT grid points,} \{N^{(0,n/\psi)}_f, N^{(f,n/\psi)}_f\}, \ s \in \text{near ion } J \)
- \( N^{(\alpha,\beta)}_f \sim 1 \) for EES interpolation.

All grid \textit{spacings} are independent of system size.

- \( N \)-ion cores in \( D(h) \): \( N_f \sim 1 \)
- \( 2R_{pc} \)
- \( R_{pc} \sim 1 \)

- Fine spherical polar grid \( (N_f) \)
- not to scale
Creating the $r$-space representation of the e-density

In the following, the multi-length scale PAW method is used to construct the electron density in $N^2 \log N$ as a demonstration:

$$n_j^{(\text{core})}(r_f) = n_j^{(\text{core 1})}(r_f) + n_j^{(\text{core 2})}(r_f) + n_j^{(S)}(r_f) \quad J = 1..N$$

$n_j^{(S)}(r)$: outside of cores

(1) Create the smooth KS states in real space, $\psi_i^{(S)}(s)$: $N^2 \log N$.
(2) Create the smooth density in real space, $n^{(S)}(s)$: $N^2$.
(3) *Create the smooth density in the ion cores, $n_j^{(S)}(r_f)$: $N \log N$.
(4) Create the smooth Z-matrix, $Z_{ij}^{(S)}$: $N^2 \log N$.
(5) *Create the core-2 densities, $n_j^{(\text{core 2})}(r_f)$: $N^2$.
(6) *Create the core-1 densities, $n_j^{(\text{core 1})}(r_f)$: $N^2 \log N$.

* New terms.

Formulae for all other components of PAW-DFT have been derived including ionic and pw expansion coefficient derivatives.
3. Creating the smooth density, $n_j^{(S)}(r_f)$ around each ion $J$, on the fine grid, $f \in N_f$

EES weighted smooth density in $g$-space

EES weighted smooth density on discrete $s$-space

EES weighted smooth density around each $J$

EES interpolated smooth density around each $J$

\[ \tilde{n}^{(S,D)}(g) = D^{(n)}(g) \, \bar{n}^{(S)}(g), \quad |g| < G_c \]

\[ n^{(S,D)}(s), \quad s \in N_{FFT}^{(n,EES)}, \quad r = hs \]

\[ n_j^{(S,D)}(s), \quad N_j^{(f,n)}: s \in \text{near } J \]

\[ n_j^{(S)}(r_f), \quad f \in N_f \]

$N$ = number of ions, $J=1..N, \quad N \neq N_{KS}$

$N_f$ = number points on spherical-polar grid around each ion.

$N_f$ and $N_j^{(f,n)}(s \in \text{near } J)$ independent system size.
Creating the $Z_{IJc}^{(S)}$ matrix for all ions of type $j_{typ}$ and channel $c$

$D^{(\psi)}(g) \tilde{p}_{j_{typ}c}^{(S)}(g)$
weighted KS states in $g$-space

1. $\text{FFT} (\psi, +, \text{EES}) \left[ \tilde{\psi}_{j_{typ}c}^{(S,D,\tilde{p})}(g), \frac{G}{2} \right]$

2. $N_{j_{typ}}$-Partition, $N_{j_{typ}}$ B-Spline Interps.

3. $Z_{IJc}^{(S)} J \in j_{typ}$

$\tilde{\psi}_{j_{typ}c}^{(S,D,\tilde{p})}(g) = D^{(\psi)}(g) \tilde{\psi}_{j_{typ}c}^{(S)}(g) \tilde{p}_{j_{typ}c}^{(S)}$
$s \in N_{FFT}^{(\psi, \text{EES})}$
$|g| < G_c/2$

$\psi_{j_{typ}c}^{(S,D,\tilde{p})}(s), s \in N_{FFT}^{(\psi, \text{EES})}$

$N_{j_{typ}}$-Partition, $N_{j_{typ}}$ B-Spline Interps.

$Z_{IJc}^{(S)} J \in j_{typ}$

$s \in \text{near ion } J^*$, of type $j_{typ}$, interpolated to obtain $Z_{IJc}^{(S)}$ for all $IJ \in j_{typ} \left( N_{B}^{(0,\psi)} \sim 1 \right)$,

$Z_{IJc}^{(S)} = \sum_{s \in \text{near } J} \psi_{j_{typ}c}^{(S,D,\tilde{p})}(s) M_{J,p}^{(3)}(s)$

$s$ independent of $I,c$ as are B splines, $M_{J,p}^{(3)}(s)$

*Note, index $J$ need not be contiguous in list of all atoms
5. Creating the core density component, $n_j^{\text{(core2)}}(r_f)$, around each ion $J$, on the fine grid, $f \in N_f$

Each KS state contributes to $N$ unique reductions

$$Z_J^{(S,2)} = \sum_I |Z_{IJ}^{(S)}|^2$$

In this example we have 1 projector

$$n_j^{\text{(core2)}}(r_f) = Z_J^{(S,2)} \Delta p^2(r_f) \forall f \in N_f$$
6. Creating the core density component, \( n_{j}^{\text{core1}}(r_f) \), around each ion \( J \), on the fine grid, \( f \in N_f \)

![Diagram showing the process of creating the core density component]

Each KS state contributes to \( N \) unique reductions  
\[
\psi_{j}^{(S,D,Z)}(s) = \sum_{l} Z_{lj} \psi_{l}^{(S,D)}(s) \quad \forall \ s \in \text{near } J: N_{B}^{(f,\psi)} \\
Z_{lj} = \text{weight for points } s \in \text{near } J \text{ from KS state, } l.
\]
PAW Charm++ Implementation Progress:

• Chare arrays defined and communication patterns established in PowerPoint form.

• Full PAW-KS-DFT flow chart for energies. Forces in progress.

• Model Charm++ software outside of OpenAtom to test fine grid spacing, Coulomb cusp smoothing, convergence with real-space cutoff, ... Complete.

• N-partition and N-consolidation operations added to charmFFT. Periodic boundary conditions need to be added.

• Ready to begin integration into OpenAtom. Maybe with new funding.
Grand Challenge Application: Perovskite solar cells

- **Pros:** High eff., low cost, tunable band gap (ABX$_3$)
- **Cons:** Instability: water, air, light, interface ... & toxic compounds.

**CH$_3$NH$_3$PbX$_3$**

- **MAI-term.**
- **Pbl$_2$-term.**
- **Pbl$_2$-defect.**

**PAW in OpenAtom**

- **Understand:** mechanism of instability/degradation.
- **Search:** non-toxic B$^{2+}$ (Fe, Co, Ni,...) for new high perf. materials.
- **Design:** new interface/encapsulation for novel devices with long lifetime.
- **System size:** 512 atoms (4x4x2 MAPbI$_3$ +128 water), 1264 states
Conclusions

• PAW-KS-DFT is an important method in computational science that allows computations beyond PW-KS-DFT – heavy atoms.

• Using EES Interpolation, we have derived a multi-length scale PAW technique that scales as $N^2 \log N$ (all energy terms and all derivatives) – an important advance and 100 pages of latex.

• Charm++ parallel framework developed; communication scaling analysis complete. Currently implementing. New funding?