Simulating Ultralight Dark Matter with Chapel

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Motivating Ultralight Dark Matter

About

- In the standard cosmological model, 80% of the matter in the Universe is "dark" (i.e. non-baryonic).
- Form gravitationally bound structures : dark matter halos.
- The traditional model is a heavy particle ($\sim 100\times$ proton), with weak interactions.

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Successes

- Explains a large scale of observations, from the rotation of galaxies, to "Bullet" clusters, to the distribution of galaxies, to the cosmic microwave background.

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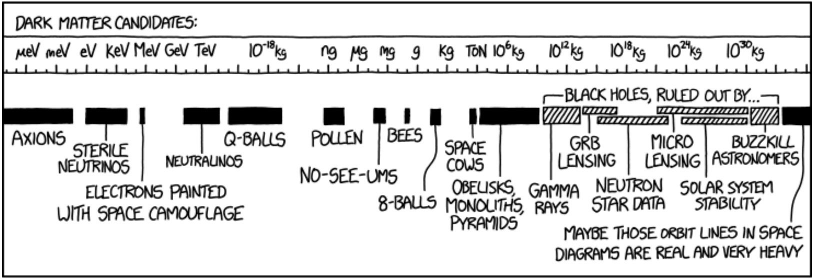
Successes

- Explains a large scale of observations, from the rotation of galaxies, to “Bullet” clusters, to the distribution of galaxies, to the cosmic microwave background.

Challenges

- Possible puzzles remain on small scales from the structure of dark matter halos, to the observed abundance of dark matter halos. Note that these might well be solved by astrophysics.
- We have not detected these in the lab, or at accelerators.



https://xkcd.com/2035

We're waaay off to the left!

Motivating Ultralight Dark Matter

- A different paradigm is a very light particle ($10^{-31}\times$ proton).
- Many names : fuzzy dark matter, Bose-Einstein dark matter, ...
- Small mass means that quantum-mechanics can smear it out over astrophysically interesting scales.
- High enough density that it forms a Bose-Einstein condensate.
- Different phenomenology : eg. interference patterns.
- Anything by the most idealized situations requires simulations.

Our Motivation

- Want a code to do numerical experiments with.
- Need scalability
  - Must resolve soliton cores : large dynamic range
  - Simulation time scales as N^5; need to scale to large numbers of nodes.
- Initial problem : revisit aspects of the formation of ultra-light dark matter halos from collisions of soliton cores.
- This is an area of very active research (we are newcomers).
- Several codes exist - including adaptive codes, codes built on existing large astrophysical simulations. Challenges to large boxes still exist.
- An incomplete list : Schive et al, 2014, Mocz et al, 2017, Edwards et al 2017, Veltmaat et al, 2018

History of Project

- `PyUltraLight`[a]: An initial code in Python, driven by Jupyter notebook
  - Easy to use and modify, allowing numerical experiments
  - Performant and multithreaded (made significant use of eg. `numexpr`, `FFTW`)
- Extending to isolated potentials hit Python bottlenecks
- Attempted a skunkworks (2019/6/22) port to Chapel for a single node. Resulting code not much longer than Python, could implement isolated potentials, better multithreaded performance.
- Distributed Code
  - Want to run larger N_{grid}, can we extend the code?
  - Isolated potential calculation led to wanting a native Chapel distributed FFT (useful for many other tasks).[b]
  - Validating the FFT led to the NAS NPB benchmark.

[a] Edwards et al, arXiv:1807.04037

[b] Note that Chapel can also interoperate with MPI.

The Schrodinger-Poisson Equations

FFTs

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + m\Phi\psi$$

$$\nabla^2\Phi = 4\pi G m|\psi|^2$$

Isolated boundary conditions

Distributed FFTs are a key component!

Slab Decompositions Are Simple

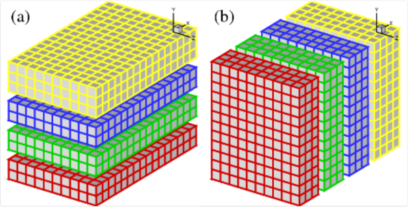


Figure: Slab Decomposition

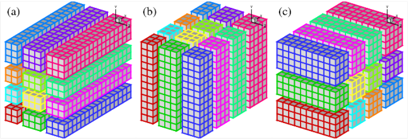


Figure: Pencil Decomposition

`http://www.2decomp.org/decomp.html`

- Slab decompositions are simpler (especially for the end user)
- Slab limits the amount of parallelism expressed (especially with pure MPI)
- Use 1 slab per locale/node.
- Limits $N_{\mathrm{grid}} \geq N_{\mathrm{nodes}}$, but in practice, not limiting.
- Reduce communication complexity

Chapel Code is Expressive : Pencil and Paper

The Algorithm

1. Decompose array into slabs in the x direction
2. Fourier transform in the y direction[a]
3. Fourier transform in the z direction
4. Transpose x and y (all to all)
5. Fourier transform in the x direction

[a] We use FFTW (`www.fftw.org`) for 1D serial transforms.

Chapel Code is Expressive : A Naive Implementation

```
coforall loc in Locales do on loc {
  ...
  for ix in xSrc {
    myplane = Src[{ix..ix, ySrc, zSrc}];
    // Y-transform
    forall iz in zSrc {
      yPlan.execute(myplane[0, ySrc.first, iz]);
    }
    // Z-transform
    forall iy in offset(ySrc) {
      zPlan.execute(myplane[0, iy, zSrc.first]);
      // Transpose data into Dst
      Dst[{iy..iy, ix..ix, zSrc}] = myplane[{0..0, iy..iy, zSrc}];
    }
  }
  allLocalesBarrier.barrier();
  // X-transform, similar to Y-transform
  ...
}
```

SPMD

Data parallel

FFTW 1D

PGAS Transpose

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    }
  }
  allLocalesBarrier.barrier();
  // X-transform, similar to Y-transform
  ...
}
```

SPMD

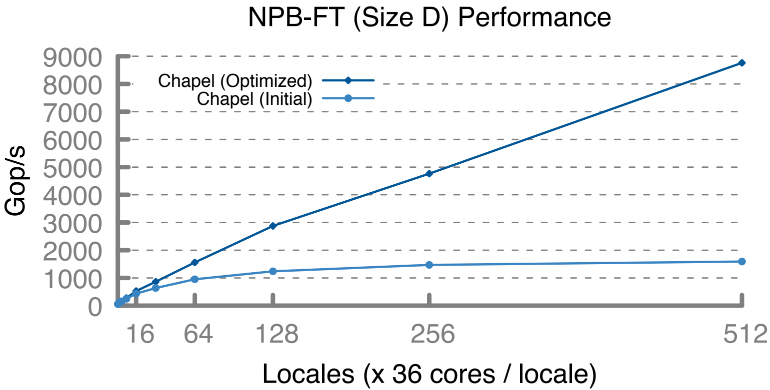
Data parallel

FFTW 1D

Reduce comm congestion!

PGAS Transpose

Chapel FFTs : Naive Performance



Chapel Code is Expressive : A Performant Implementation

overlap computation and comm

```
...
forall iy in offset(ySrc) {
  zPlan.execute(myplane[0, iy, zSrc.first]);
  // Transpose data into Dst, and copy the next Src slice into myplane
  copy(Dst[...], myplane[...], myLineSize);
  if (ix != xSrc.last) {
    copy(myplane[...], Src[...], myLineSize);
  }
}
...
```

low-level comm

batch FFTW calls (not shown)

Benchmarks

Machine/Compiler Specifications

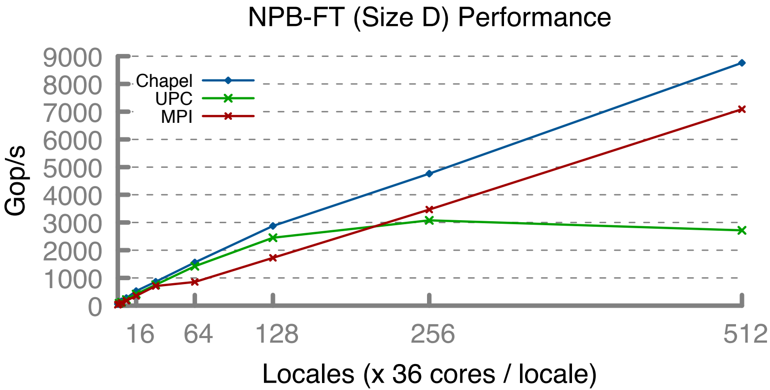
- Scalability Hardware (Cray-XC):
  - 36-core (72 HT), 128 GB RAM
  - dual 18-core (36 HT) ”Broadwell” 2.1 GHz processors
- Software
  - CLE 7.0.UP01
  - Intel Compilers 19.0.5.281
  - FFTW 3.3.8.4
  - Chapel 1.20.0
  - Cray 9.0.2 (classic)

Benchmarks

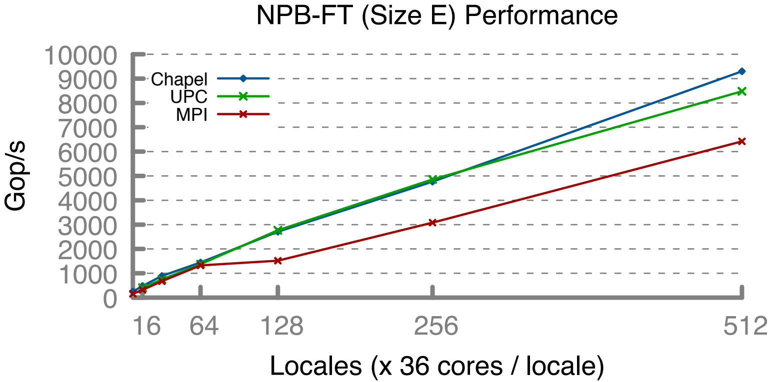
Benchmarks

- Use the NAS NPB-FT benchmark
  - NPB v3.4
  - Class D ($2048 \times 1024 \times 1024$), E ($8\times$), F($8\times$)
- Compare Chapel, MPI reference and UPC (with non-blocking overlapped comm)
- MPI and UPC use pencil decompositions for large problems/node counts.
- MPI and UPC use 32 cores/node (require a power of 2)
  - Restricting Chapel to 32 cores dœs not significantly change timings, indicating memory/communication bound.

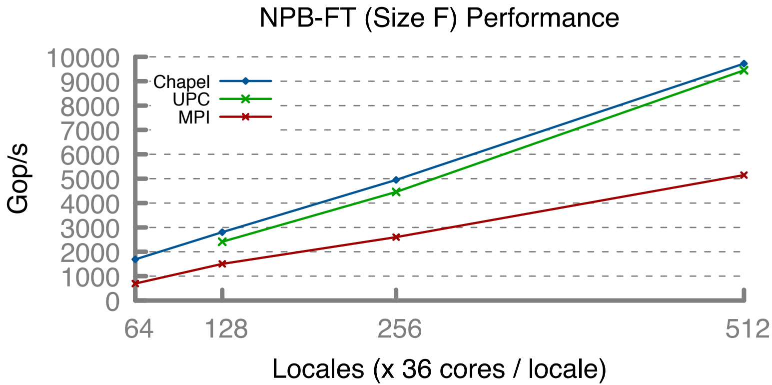
Chapel FFTs Scale Well Across Nodes : Class D



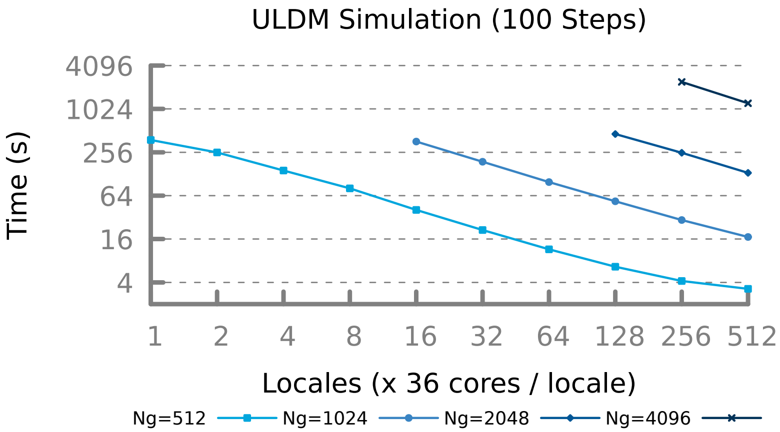
Chapel FFTs Scale Well Across Nodes : E = 8×D



Chapel FFTs Scale Well Across Nodes : F = 8×E



Simulations Scale Well



Writing a Research Code

Plumbing

- Parallel HDF5 for saving full simulations (interop with MPI)
- HDF5 Tables for serializing arrays of records
- (C)TOML for input parameters

All of the above are good examples of C interop.

Analysis

- Summary statistics run in-line; need to be fast.
- eg. Density/Energy profiles/histograms

These get modified often; do not want to introduce a bottleneck.

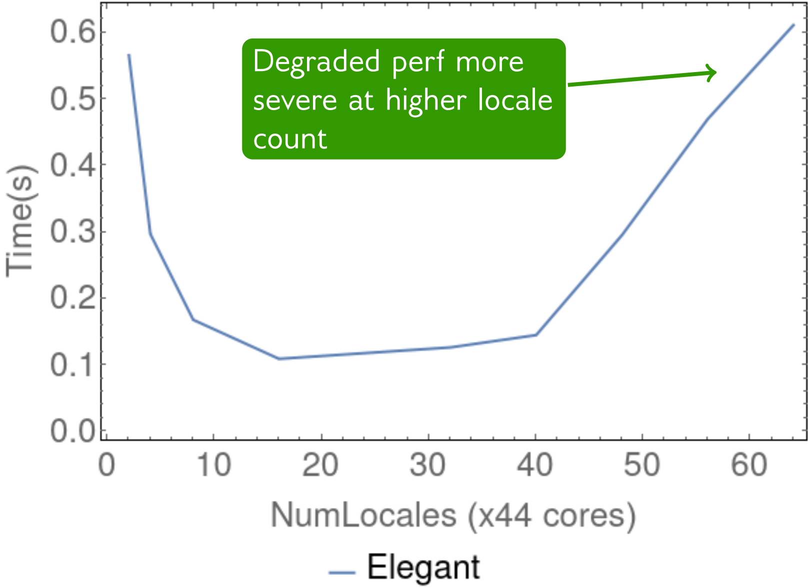
Computing Density Profiles/Histograms : Elegant

'Dom' is a distributed domain

```
var counts : [ProfDom] real;
forall (i,j,k) in Dom with (+ reduce counts) {
  const rr = sqrt(i*i + j*j + k*k):int;
  counts[rr] += 1.0;
}
```

That's elegant!

Timings : Elegant



Computing Density Profiles/Histograms : Atomic

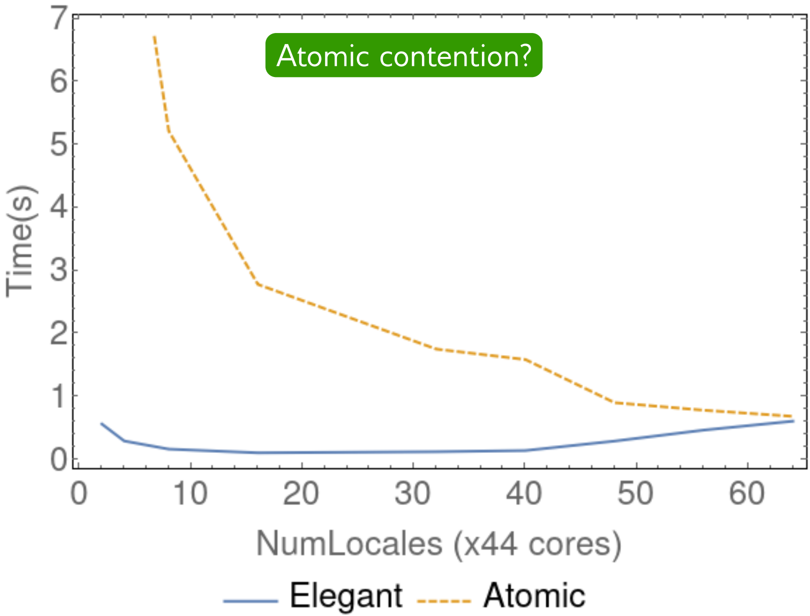
Local counts

Avoid network atomics

```
var priv_counts : [PrivateSpace][ProfDom] chpl__processorAtomicType(real);
var counts : [ProfDom] real;
forall (i,j,k) in Dom  {
  const rr = sqrt(i*i + j*j + k*k):int;
  priv_counts[here.id][rr].add(1.0);
}
for iloc in 0.. #numLocales {
  var loc_counts = priv_counts[iloc];
  forall ii in ProfDom do counts[ii] += loc_counts[ii].read();
}
```

Manual reduction

Timings : Atomic

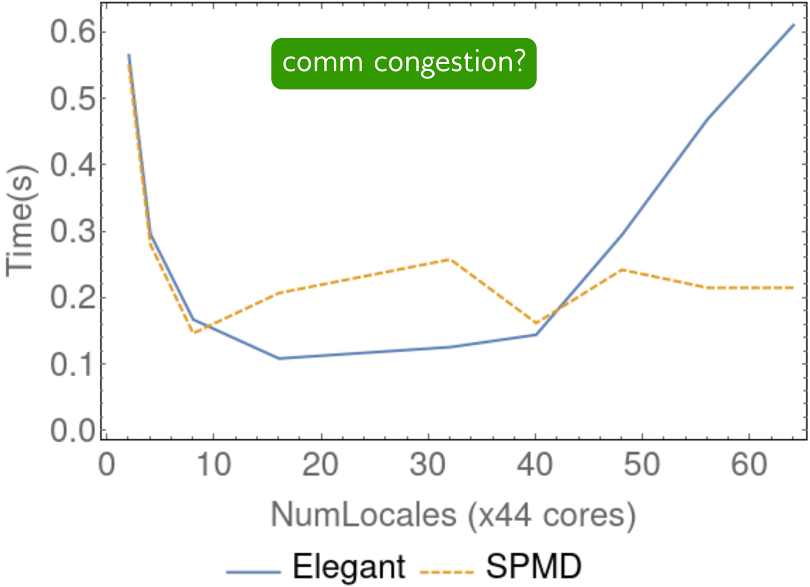


Computing Density Profiles/Histograms : SPMD

```
var priv_counts : [PrivateSpace][ProfDom] real;
var counts : [ProfDom] real;
coforall loc in Locales do on loc {
    const myDom = Dom.localSubdomain();
    ref mycounts = priv_counts[here.id];
    forall (i,j,k) in myDom with (+ reduce mycounts) {
      const rr = sqrt(i*i + j*j + k*k):int;
      mycounts[rr] += 1.0;
    }
  }
for iloc in 0.. #numLocales {
  var loc_counts = priv_counts[iloc];
  forall ii in ProfDom do counts[ii] += loc_counts[ii];
}
```

SPMD, local reduction

Timings : SPMD

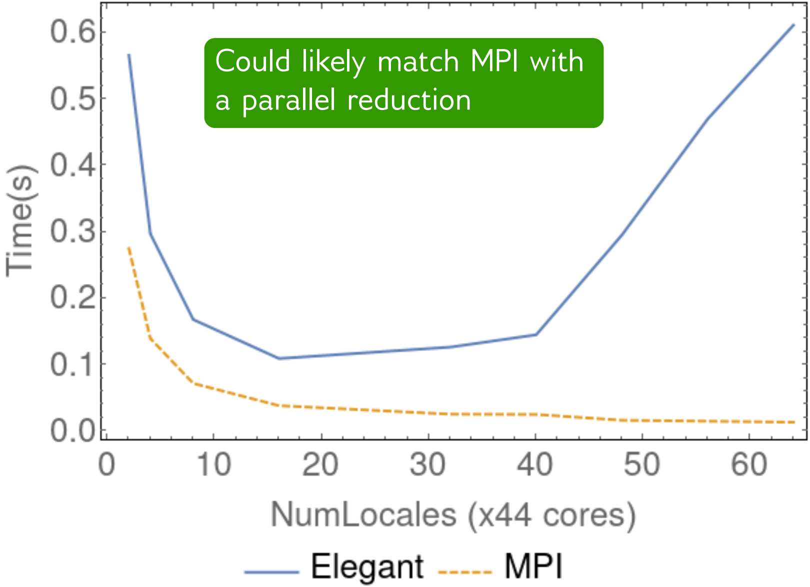


Computing Density Profiles/Histograms : MPI

```
var counts : [ProfDom] real;
coforall loc in Locales do on loc {
    const myDom = Dom.localSubdomain();
    var mycounts, recvbuf : [ProfDom] real;
    forall (i,j,k) in myDom with (+ reduce mycounts) {
      const rr = sqrt(i*i + j*j + k*k):int;
      mycounts[rr] += 1.0;
    }
    MPI.Barrier(CHPL_COMM_WORLD);
    if (here.id==0) {
      MPI_Reduce(mycounts[0], recvbuf[0], (2*Ng):c_int,
                 MPI_DOUBLE, MPI_SUM, 0, CHPL_COMM_WORLD);
      counts = recvbuf;
    } else {
      MPI_Reduce(mycounts[0], recvbuf[0], (2*Ng):c_int,
                 MPI_DOUBLE, MPI_SUM, 0, CHPL_COMM_WORLD);
    }
  }
```

Use MPI if needed

Timings : MPI


Could likely match MPI with a parallel reduction
Time(s)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
10
20
30
40
50
60
NumLocales (x44 cores)
Elegant
MPI

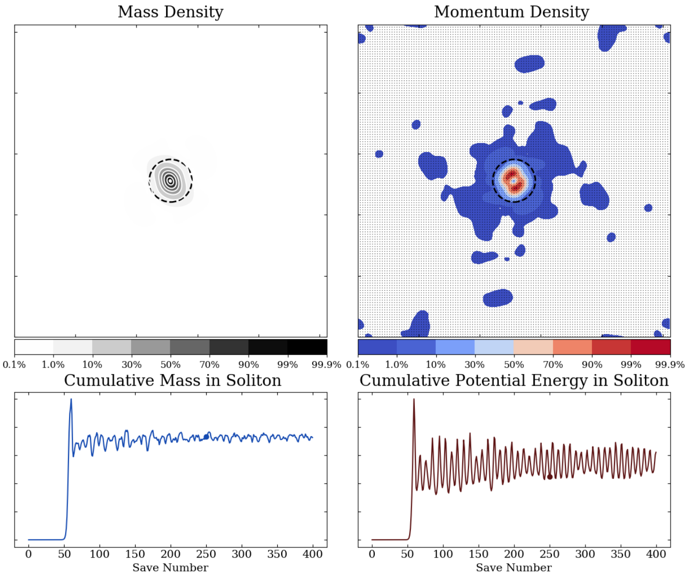
Science, Powered by Chapel

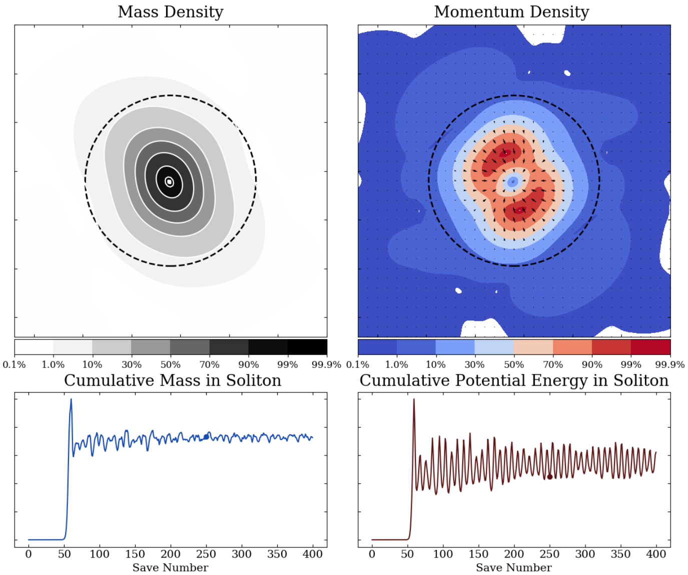
In Active Use

- Actively being used by Luna Zagorac for her thesis.
- All plots/movies are courtesy Luna, simulations are Chapel powered!
- Code is being actively developed, with new science modules being added in!

Binary Collisions

- Cosmological structures form hierarchically.
- Run simulations colliding pairs of solitons, exploring different initial conditions.
- Final state of system?
- Time scales involved?


Mass Density
Momentum Density
0.1% 1.0% 10% 30% 50% 70% 90% 99% 99.9%
0.1% 1.0% 10% 30% 50% 70% 90% 99% 99.9%
Cumulative Mass in Soliton
Cumulative Potential Energy in Soliton
0 50 100 150 200 250 300 350 400
Save Number
0 50 100 150 200 250 300 350 400
Save Number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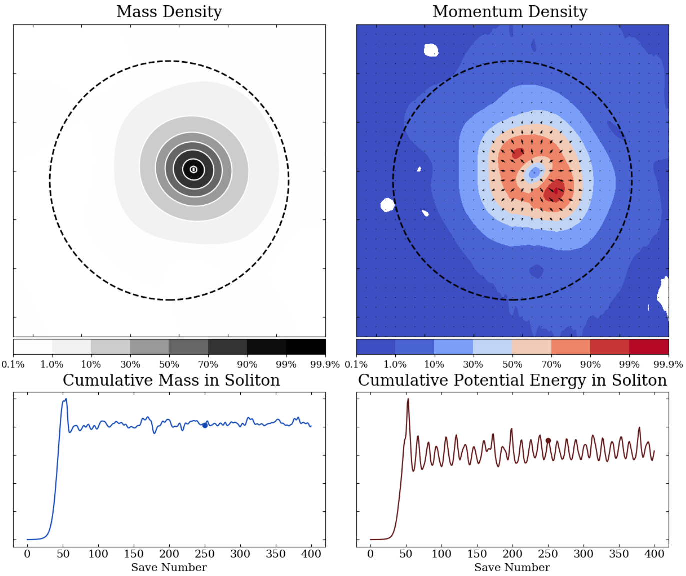
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Where Chapel could do better

1. Tooling
   - Identifying communication - how much and from where? How to recognize a sub-optimal pattern.
   - Easier profiling
   - Compiler improvements, including speed.
2. Easier to express low-level communication/locality
   - Low level communication primitives are not exposed to user (useful when the user can reason better about the communication patterns).
   - Verbose to express locality of computation and have the compiler optimize appropriately.
3. Fewer hidden performance traps
   - Unexpected communication
   - Promotion of operations over N-d arrays can be slow.

None of these are new issues to the Chapel team (and many have Github issues).

My Thoughts

- HPC:
  - *Productivity*: Chapel design has scientific codes in mind.
    - Domains/Arrays
    - Expressive Parallelism - where/when you need it.
    - Interoperability - C (and now Python!)
  - *Performance*: Chapel code can perform/scale very well without heroic efforts.
- It's a fun language to write. Easy to throw together prototype code in. And it largely dœs the right thing!
- I'm getting to the point where I'm just working in Chapel.