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Improvements to a free-space FFT Poisson solver in the Independent Parallel Particle Layer

Master thesis

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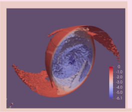
Overview

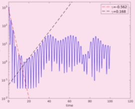
OPAL and IPPL

ALPINE: A set of portable pLasma physics Particle-in-cell mINi-apps for Exascale

Two-stream Instability | Penning trap | Landau damping

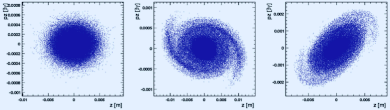
- Light weight codes
- Proxy for real applications
- For implementing new algorithms
- Testing new implementations
- Reference results ensure correctness





OPAL: Object oriented Parallel Accelerator Library

Open source C++ Library for particle accelerators being developed by twelve core developers across seven institutes



Source: OPAL web page

Independent Parallel Particle Layer (IPPL) v 2.0

- FFT based Poisson Solver
- CG
- heFFTe
- D-Operators
- Interpolation
- Fields
- Mesh
- Particles
- Load Balancing
- Domain Decomp.
- Communication
- Buffer factory
- MPI
- Kokkos

Introduction: Problem to solve as in OPAL

Adelmann et al. (2019)

Poisson equation: $\Delta\phi = \rho$.

$\rightarrow$ Can write the solution as a convolution:

$$\boxed{\phi(\vec{r}) = (G * \rho)(\vec{r}) = \int G(\vec{r} - \vec{r}')\rho(\vec{r}')d\vec{r}'}$$

$\implies$ can use **FFT-based** methods

$$\phi = h_x h_y h_z \mathrm{FFT}^{-1}\{\mathrm{FFT}\{\rho\} \cdot \mathrm{FFT}\{G\}\}$$

Periodic Boundary Conditions
$\rightarrow$ Can use directly

Open Boundary Conditions
$\rightarrow$ Make periodic (Hockney and Eastwood, 1988)

A novel method for Open boundaries: Vico et al. (2016)

Based on the standard Hockney trick (Hockney and Eastwood, 1988)

Hockney and Eastwood (1988)

- Double the domain $\implies (2N)^3$.
- On doubled grid, make periodic $\implies \rho_2, G_2$.
- Use FFT to compute convolution.
- Restrict solution to the physical domain.

Vico et al. (2016)

Green's function in Fourier space:

$$G_L(\vec{s}) = 2\left(\frac{\sin(L|\vec{s}|/2)}{|\vec{s}|}\right)^2,$$

where $L > \sqrt{L_x^2 + L_y^2 + L_z^2}$ is the length of the truncation window.

Motivations

Problem

G Requires **pre-computation** on a $4N^3$ grid to satisfy sampling theorem.

Large memory footprints $\implies$ Inability of running large problems, especially on GPUs.

Solution

Exploit symmetry of G around its $2N+1$-th element. Instead of inverse-FFT on a domain of size $4N^3$, pre-compute G with an inverse DCT.

$\rightarrow$ domain size reduced to $2N^3$.

DCT definition and choice

DCT $\equiv$ DFT of twice the length operating on periodic and symmetric coefficients.

To fit the location of the symmetry centre, we want type I.

$$Y_k = \frac{1}{2(N-1)}\left(x_0 + (-1)^k x_{N-1} + 2\sum_{n=1}^{N-2} x_n \cos\left[\frac{\pi k n}{N-1}\right]\right)$$

Discrete Cosine Transforms in heFFTe

Native implementation

Only one back-end providing it

Non-native implementation

Rely on R2C and C2R backward and forward transforms, with the help of pre and post processors to match the transform type.

Non-native implementation: algorithm

`inputData` ← data to be transformed

`inputExtended` ← `preProcessingKernel(inputData)`

`outputComplex` ← `R2C(inputExtended)`

`outputReal` ← `postProcessingKernel(outputComplex)`

cuFFT DCT-I implementation

Intuition

Taken a signal x of length N, it is possible to construct its DCT-I through a real to complex DFT.

1. Construct the signal y, of length $4(N-1)$, such that:

$$y[n]_{n\in[0,\ldots,4(N-1))} = \begin{cases} x[n/2], & \text{if } n \text{ even and } n \leq 2N \\ x[(4(N-1)-n)/2] & \text{if } n \text{ even and } 2N < n < 4(N-1) \\ 0.0 & \text{otherwise} \end{cases}$$

2. Perform a DFT on the extended signal, which will result in:

$$Y[k] = \frac{1}{4(N-1)} \sum_{n=0}^{4(N-1)-1} y_n e^{\frac{-2\pi ikn}{4(N-1)}}$$

cuFFT DCT-I implementation

Intuition: cont'd

3. Re-write in terms of x :

$$= \frac{1}{4(N-1)}\left[e^{0}x_0 + e^{-\pi ik}x_{N-1} + \sum_{n=1}^{N-2} x_n\left(e^{\frac{-2\pi ik2n}{4(N-1)}} + e^{\frac{-2\pi ik(4(N-1)-2n)}{4(N-1)}}\right)\right]$$

$$= \frac{1}{4(N-1)}\left[x_0 + (-1)^k x_{N-1} + \sum_{n=1}^{N-2} x_n\left(e^{\frac{-\pi ikn}{N-1}} + e^{\frac{\pi ikn)}{N-1}}e^{-2\pi ik}\right)\right]$$

$$= \frac{1}{2(N-1)}\left[x_0 + (-1)^k x_{N-1} + 2\sum_{n=1}^{N-2} x_n \cos\left[\frac{\pi kn}{N-1}\right]\right]$$

Which is the definition of the (normalized) DCT of type I.

cuFFT DCT-I implementation

Adjustments

Use these steps to write the processing kernels.

Theoretically, kernels should be the same independently from type of transform (forward/backwards), since $DCT\text{-I}^{-1} = DCT\text{-I}$.

In reality, they have minor differences to fit cuFFT data types.

FFT type	Input size	Output size
C2C	N *cufftComplex*	N *cufftComplex*
C2R	$\lfloor \frac{N}{2} \rfloor + 1$ *cufftComplex*	N *cufftReal*
R2C	N *cufftReal*	$\lfloor \frac{N}{2} \rfloor + 1$ *cufftComplex*

cuFFT DCT-I implementation

Forward kernels

Pre forward

```
// DCT-I (REDFT00)
// even symmetry and periodicity;
//(a b c d) -> (a 0 b 0 c 0  d  0 c 0 b 0)
```

$4(N - 1)$ Real numbers

Pre backward

```
// IDCT-I backward kernel for DCT-I.
// set imaginary parts to zero; even symmetry
// (a b c d) -> (a+0i b+0i c+0i  d+0i  c+0i b+0i 0+0i)
```

$2N - 1$ Complex numbers $\rightarrow 4N - 2$ floating-point numbers.

cuFFT DCT-I implementation

Forward kernels

Post backward/forward kernels

```
void cos1_post_backward_kernel(int N, scalar_type const
     *fft_signal, scalar_type *result){
    int ind = blockIdx.x*BLK_X + threadIdx.x;
    if(ind < N){
        result[ind] = fft_signal[2*ind];
    }
}
```

In the case of post processing kernels, code is the same but mathematical meaning is different.
Forward → extracts real part out of complex vector.
Backward → extracts even coefficients out of real vector.

Improved Vico: algorithm

Extend ρ to ρ_{2N} on $(2N)^3$ grid.

↓

Pre-compute $G_{2N+1} \leftarrow$ Vico Green's function up to the $2N+1$-th point (up to centre of symmetry).

↓

Compute $DCT^{-}1\{G_{2N+1}\}$ and restrict $G_{2N+1} \rightarrow G_{2N}$ to $(2N)^3$ grid.

↓

Solve Poisson via convolution
$\phi = h_x h_y h_z \mathrm{FFT}^{-1}\{\mathrm{FFT}\{\rho_{2N}\} \cdot \mathrm{FFT}\{G_{2N}\}\}$

Improved Vico

Testing Setup

Test case

Gaussian test (Mayani, 2021)

Runs a single iteration of the solver with a Gaussian source.

Grid points = from 64^3 until memory overflow for the non-optimized case is met.

Architecture

Single CPU node from the **Merlin** cluster at PSI.

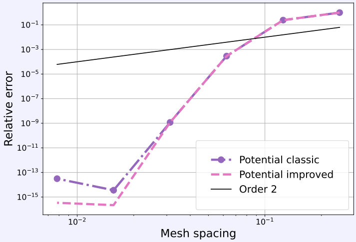
$\rightarrow$ Two Intel Xeon Gold 6152 (44 CPUs, 380GB).

Memory tracker: **Kokkos Memory Highwater.**

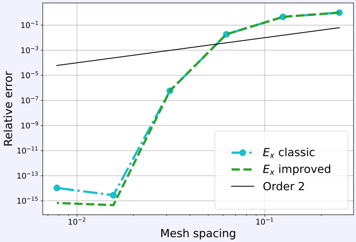
Improved Vico

Accuracy

Potential field



Electrostatic field



Correctness is verified for the improved method.

We now have better accuracy than the state-of-the-art Hockney (Order 2) without losing to it in memory footprint.

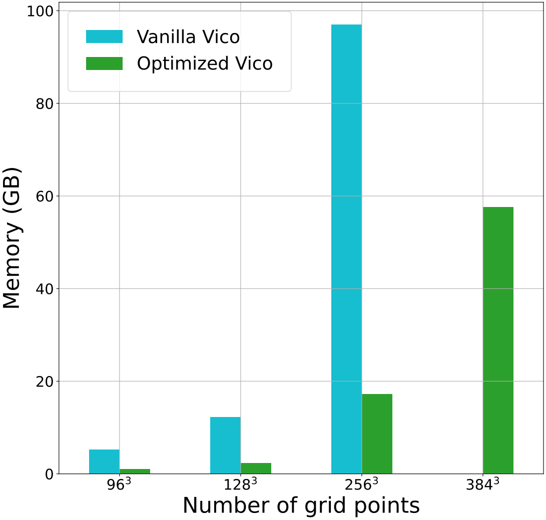
Improved Vico

Memory results

Possible to fit **more problem sizes** $< 512^3$ in a single node **with the optimized version**.

Highwater tracked a memory saving of $[\mathbf{70\%} \div \mathbf{80\%}]$.

Theoretical memory footprint reduction ≈ 8



Next steps

heFFTe

- GPU benchmarking for DCT-I
- Finalize DST-I kernels for sake of completeness
- Add kernels for CPU
- Test mixed-precision communication

IPPL

- Test mixed-precision communication
- Find and fix bug in GPU execution space
- GPU and CPU benchmarking
- Memory study on GPU

Next steps: heFFTe

Testing mixed-precision communication

Goal

Test the accuracy of the mixed precision communication currently being implemented in heFFTe.

$\rightarrow$ Choose physics-based candidate application from IPPL for testing.

Candidate application

Gaussian convergence test with Hockney solver.

$\Longrightarrow$ Well-studied physical solution to check the results.

$\Longrightarrow$ Converges at second order, more accuracy is not needed.

Next steps:IPPL

GPU bug hunting

Problem

`Solver` class fails with any R2R transform when executed on GPU (not only DCT-I).

Checks:

R2R transforms specialised class	FFT transform	Solver class
✓	✓	X

Aknowledgements

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References

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