2DECOMP&FFT – A Highly Scalable 2D Decomposition Library and FFT Interface

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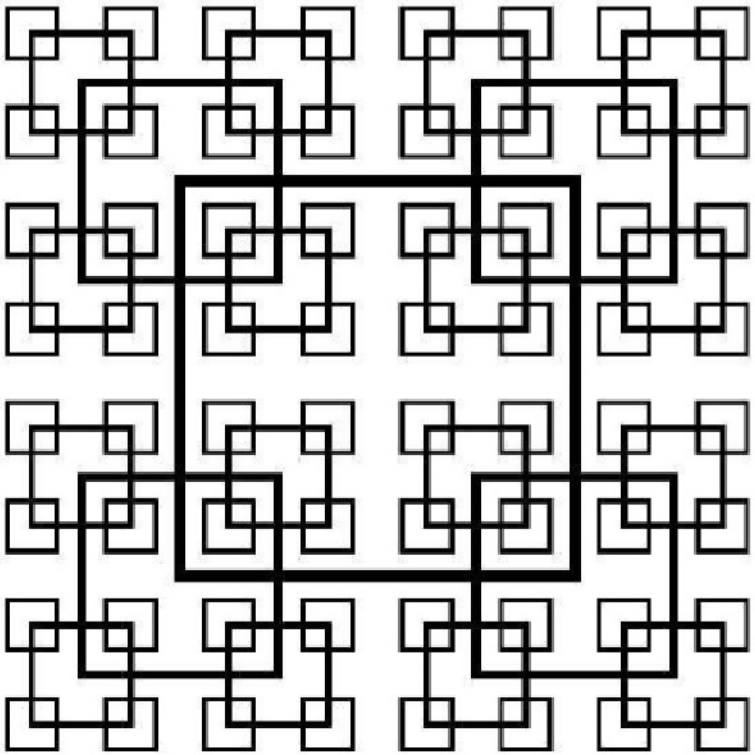
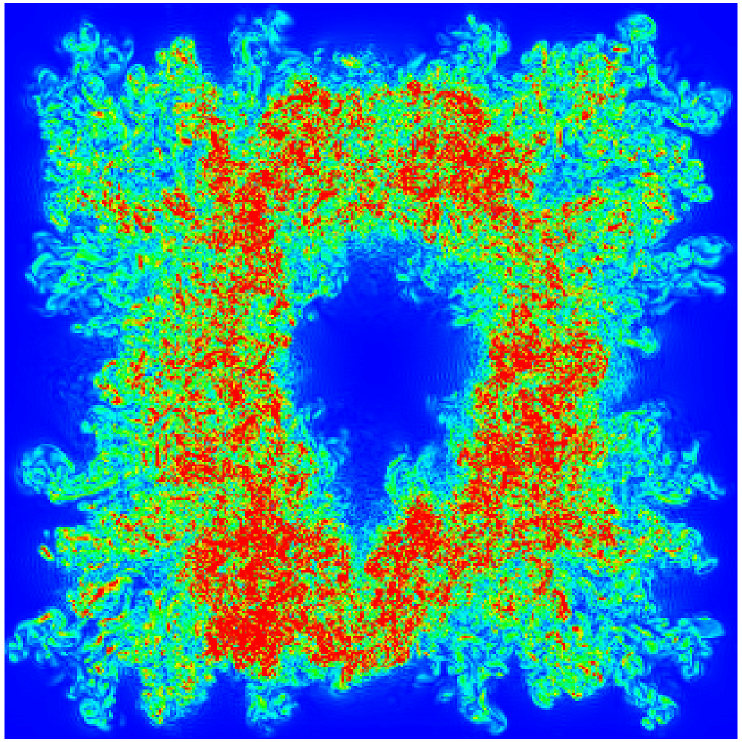
Background Information

- HECToR dCSE project ongoing
  - dCSE - dedicated software engineering support to UK research community
  - Support Imperial-based Turbulence, Mixing and Flow Control group, improving a CFD code Incompact3D
  - Opportunities identified to develop reusable software components for a wider range of applications
- Parallel library development
  - A general-purpose 2D decomposition library
    - For applications based on 3D Cartesian data structures
  - A distributed 3-dimensional FFT library
  - A distributed FFT-based Poisson solver

Scientific Applications





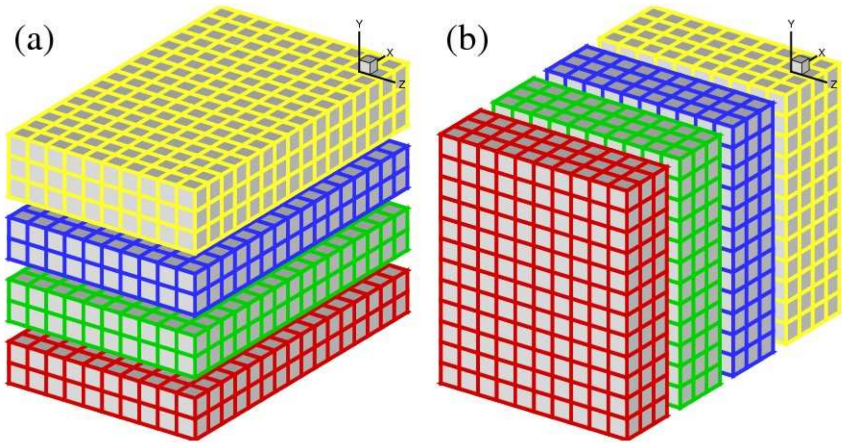
- Flow passing through multi-scale fractal grid
- Energy-efficient way to generate turbulence
- Very fine grid (~billions) required for such simulations

Algorithms and Parallel Solutions

- Incompact3D uses
  - Compact Finite Difference method → $af'_{i-1}+bf'_{i}+cf'_{i+1} = RHS$
  - Pressure Poisson solver → 3D FFT → multiple 1D FFTs
  - All values along a global mesh line involved
- General parallel solutions
  - Parallelise the elementary algorithms
    - Distributed tri-diagonal solver
    - Distributed 1D FFT
  - Redistribute the data among multiple domain decompositions
    - Often the preferred method
    - Well-developed serial algorithms can be kept unchanged

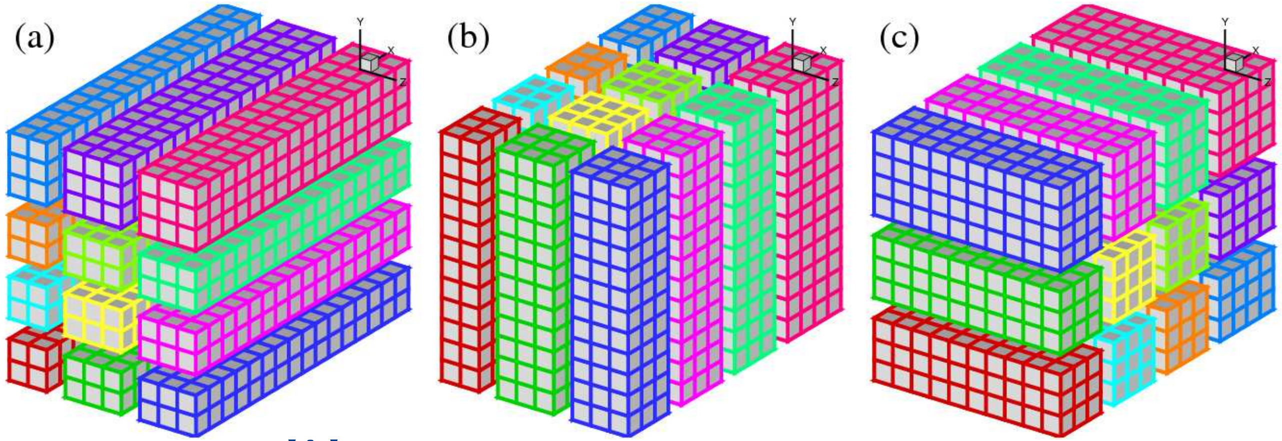
1D Decomposition

- Two slab decompositions
- Procedure
  - (a) operate locally in X, Z
  - Transpose to state (b)
  - (b) operate locally in Y
  - Transpose back to state (a)
- Limitation
  - For N^3 mesh, N_proc < N
  - Also memory limit



Typical Incompact3D simulation
2048*512*512
N_proc < 512
On HECToR
200,000 time steps at 4 seconds each
25 days wall-clock time
(excluding queueing time)

2D Decomposition



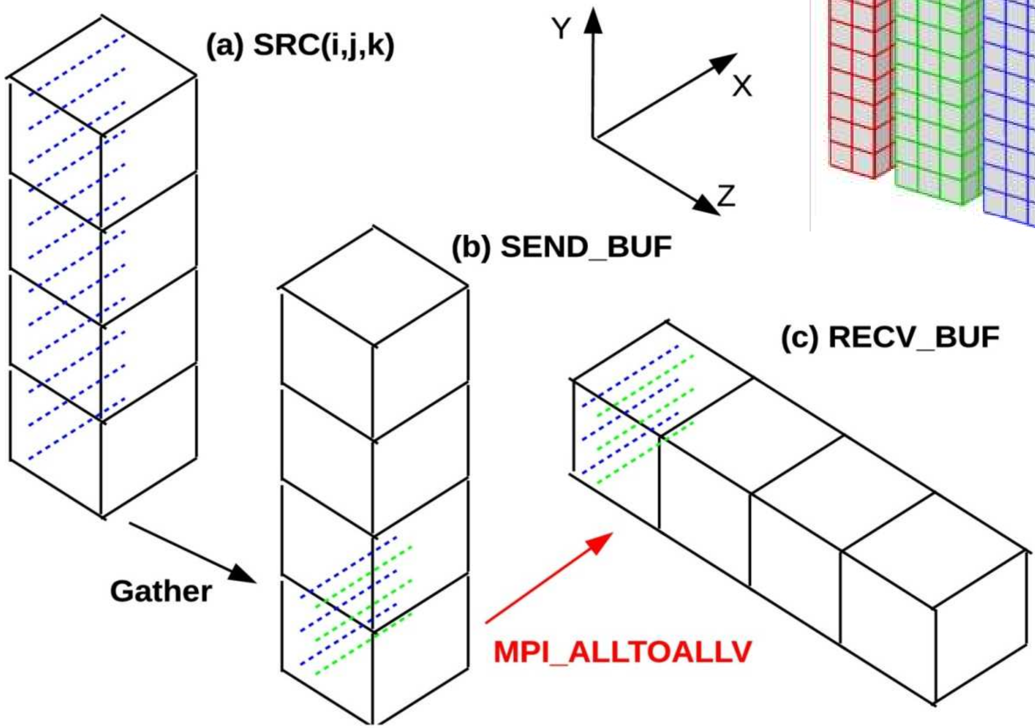
- 2D Decomposition
  - Also known as **pencil** or **drawer** decomposition
  - Local operations in one direction at a time
  - Transpose
    - (a) ⇔ (b) ⇔ (c) ⇔ (b) ⇔ (a)
    - Communication among sub-groups only
  - Constraint relaxed to N_proc < N^2 for cubic mesh

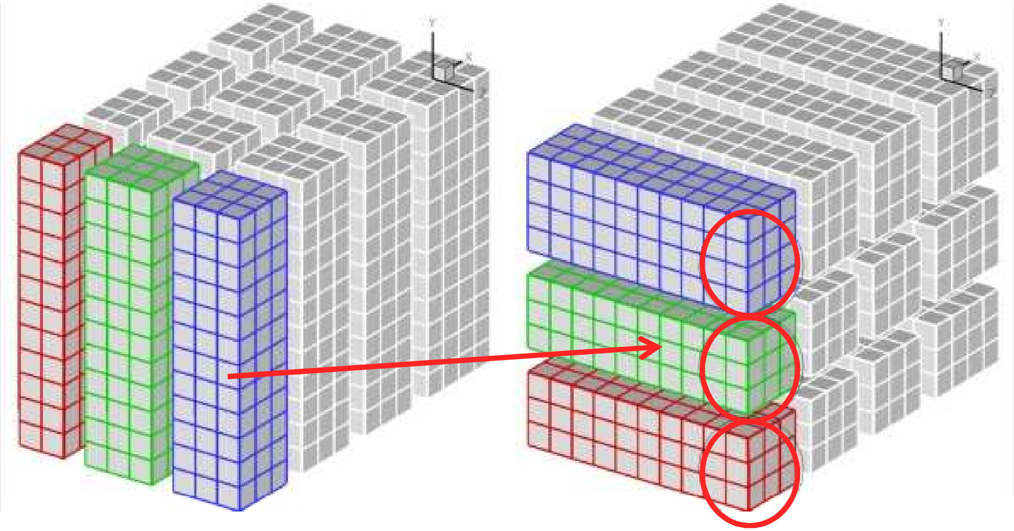
Why a Library Solution?

- Many applications.
- For a given global data structure and a given domain decomposition strategy, the corresponding data movement strategy should be identical.
- The implementation is a purely software engineering issue (not relevant to the scientific topics being studied).
- The proper implementation is not easy but important for performance reason.

Transpose from Y-pencil to Z-pencil

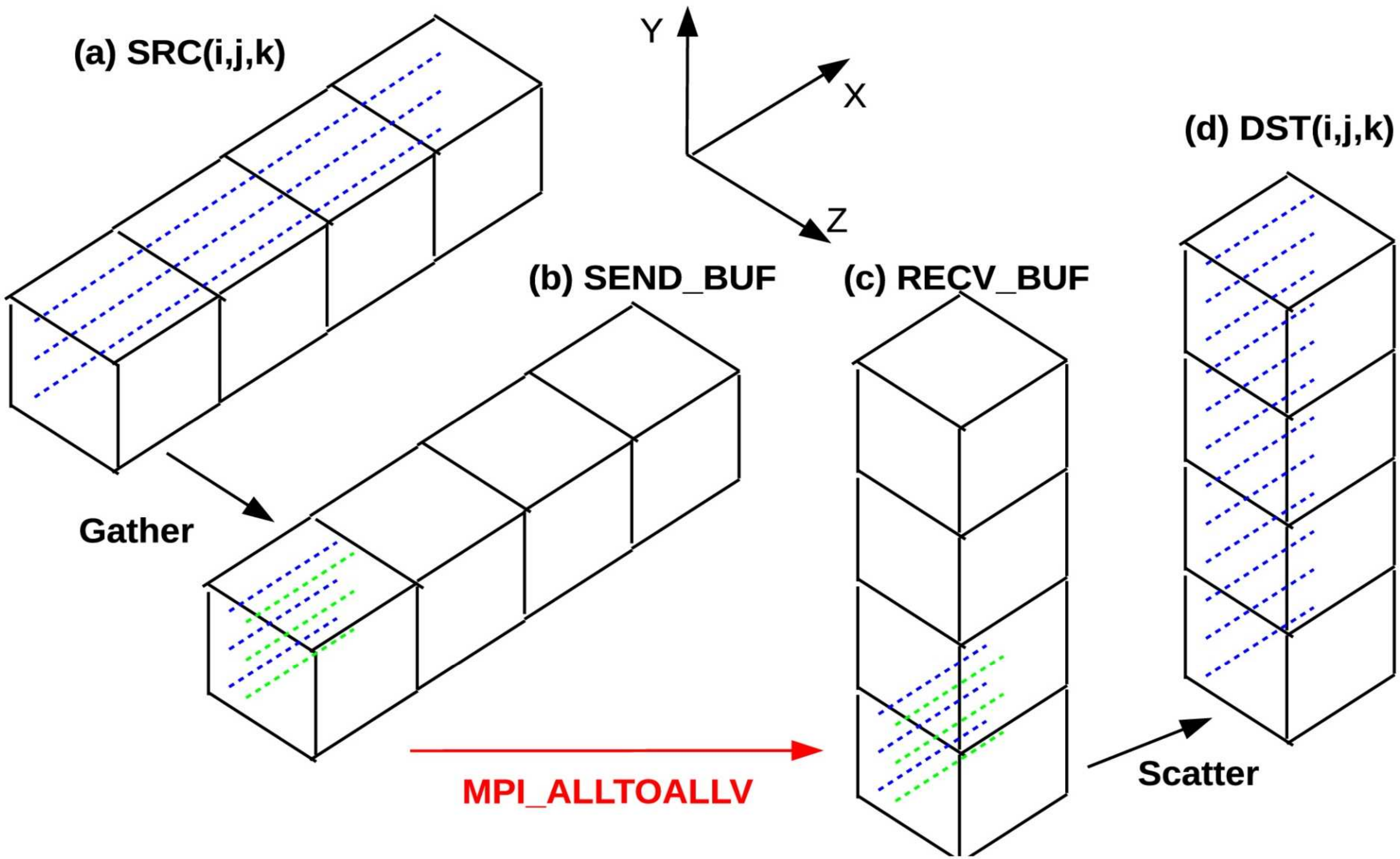
MPI_ALLTOALLV(sendbuf, sendcounts, sdispls, sendtype, recvbuf, recvcounts, rdispls, recvtype, comm)





- Best buffer gathering / scattering strategy?
- Optimisation opportunity?

Transpose from X-pencil to Y-pencil



Decomposition API

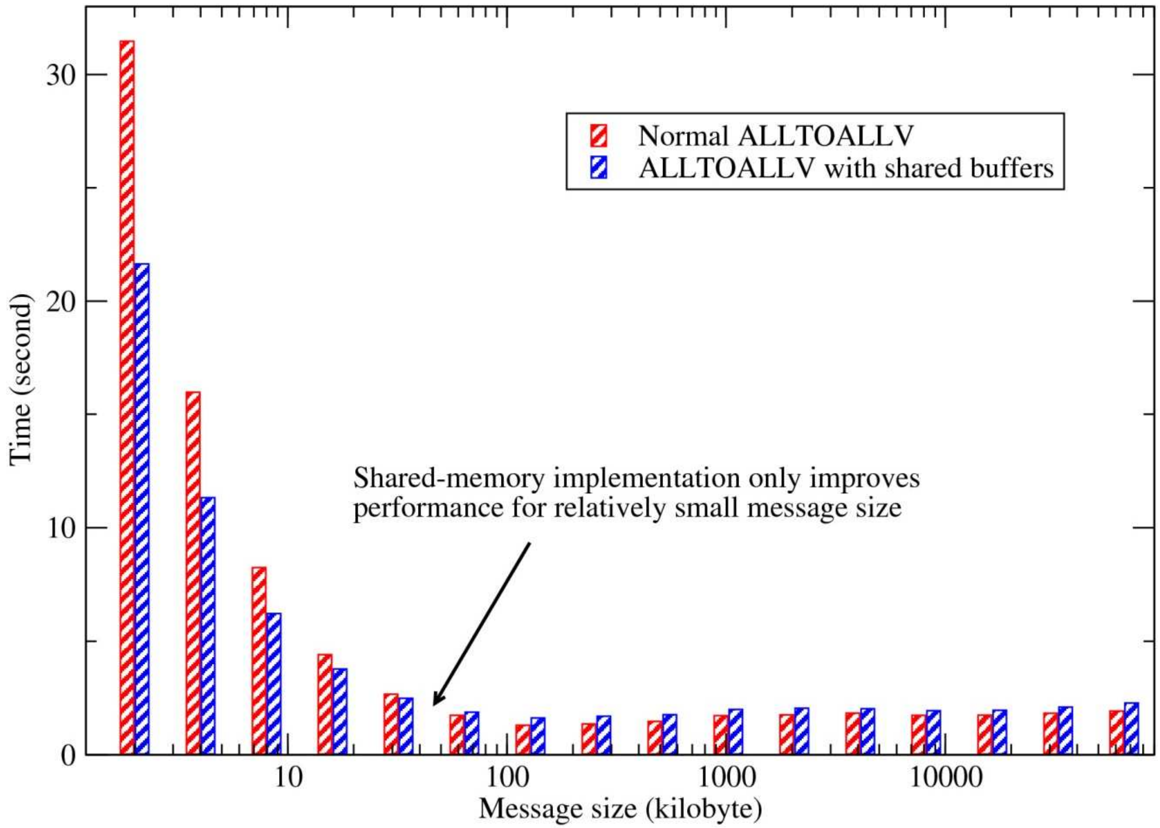
- Fortran module
  - **`use decomp_2d`**
- Global variables
  - Starting/ending index and size of the sub-domain held by current rank, required to define application data structures
    - **`allocate(in(xsize(1),xsize(2),xsize(3))`**
    - **`allocate(out(ystart(1):yend(1), ystart(2):yend(2), ystart(3):yend(3))`**
- Public subroutines
  - **`decomp_2d_init(nx,ny,nz,p_row,p_col)`**
  - **`transpose_x_to_y(in,out); transpose_y_to_z(in,out)`**
  - **`transpose_z_to_y(in,out); transpose_y_to_x(in,out)`**
  - **`decomp_2d_finalize`**

Shared-memory Implementation

- ALLTOALL(V) can be very expensive.
- Supercomputers prefers a small number of large messages.
- HECToR has 8GB memory shared by 4 cores.
- Cores on same node copy data to/from shared buffers.
- Only leaders of the nodes participate in communications.

- Implemented using System V IPC shared-memory API.
- Transparent to applications (switch on by a compiler flag).
- Originally based on Cray's code (D. Tanqueray).
- Portable implementation using Ian Bush's FreeIPC.

Shared-memory Performance



- Performance improvement for smaller message size
- Potential on next-generation hardware (24-core HECToR)

Overview of Distributed FFT Libraries

FFT Library	Comments
FFTW 2.x	MPI interface with 1D decomposition
FFTW 3.x	α-version MPI interface
CRAFFT (xt-libsci)	Evenly distributed 1D decomposition
Plimpton's parallel FFT# *	Complex-to-complex transforms only
Takahashi's FFTE #	Evenly distributed data; small prime factors
P3DFFT #	Real-to-complex/complex-to-real transforms only

- # based on 2D decomposition
- * user-callable communication routines
- All with some limitations
- Having developed the underlying decomposition library, building a distributed FFT library on top is easy

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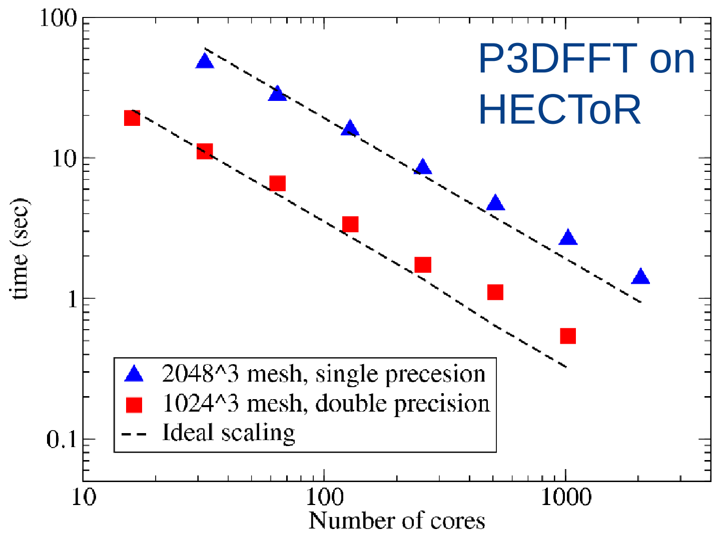
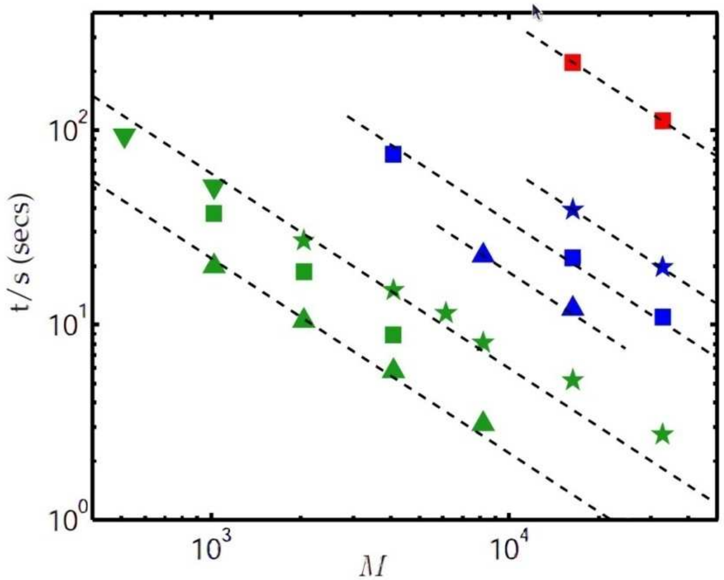
P3DFFT

- P3DFFT
  - Open-source software by Pekurovsky (SDSC)
  - Only r2c/c2r transforms
  - Private data transposition routines
- Application
  - Turbulence research using spectral DNS code by Yeung, *et al.*
  - Internally using P3DFFT
- Aim to achieve at least similar scaling





Distributed FFT API

- Fortran module
  - use decomp_2d_fft
- Public subroutines
  - decomp_2d_fft_init
    - By default, physical space in X-pencil, spectral space in Z-pencil
    - Optional parameter to use the opposite
  - decomp_2d_fft_3d (generic interface)
    - (complex in, complex out, direction) complex to complex
    - (real in_r, complex out_c) real to complex
    - (complex in_c, real out_r) complex to real
  - decomp_2d_get_fft_size (allocate memory for c2r/r2c)
  - decomp_2d_fft_finalize

Implementing Distributed FFTs

- Complex to complex (c2c) -- easy
  - Update decomposition routines to support complex data type (Fortran generic interface)
- Real-to-complex (r2c) and complex-to-real (c2r)
  - Data storage considering conjugate symmetry
  - For nx real input r_k, the complex output: $c_k = a_k + ib_k$
    - (1) also nx real numbers (Hermitian storage)
    - (2) nx/2+1 complex numbers – **easier to extend to multi-dimension**

	r1	r2	r3	r4	r5	r6	r7	r8
	c1	c2	c3	c4	c5	c6=$\underline{\text{c4}}$	c7=$\underline{\text{c3}}$	c8=$\underline{\text{c2}}$
(1)	a1	a2	a3	a4	a5	b4	b3	b2
(2)	c1	c2	c3	c4	c5	--	--	--

Extension of Base Communication Library

- Requirement
  - FFT real input: nx*ny*nz; complex output: (nx/2+1)*ny*nz
  - Both need to be distributed as 2D pencils
- Solution
  - Object-oriented style design
  - Store decomposition information per global size in a Fortran derived data type
    - Containing sub-domain sizes; starting/ending indices; Mesh distribution and MPI_ALLTOALLV buffer parameters; etc.
    - `TYPE(DECOMP_INFO) :: decomp`
    - `call decomp_info_init(nx,ny,nz,decomp)`
  - Optional third parameter to transposition routines
    - `call transpose_x_to_y(in,out,decomp)`

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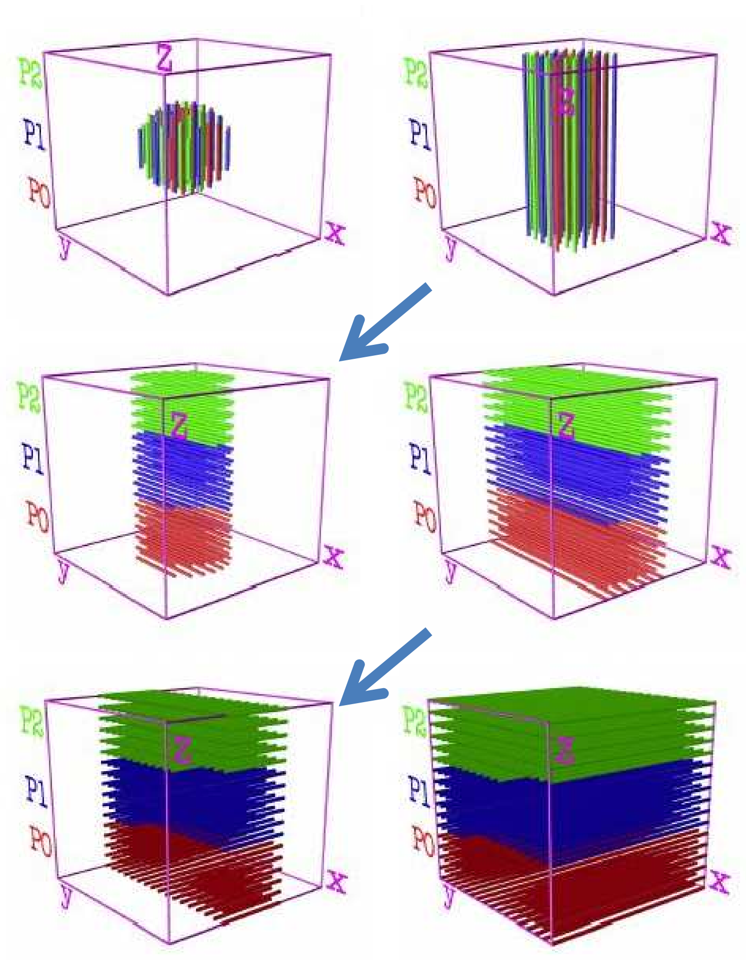
Other Multi-global-size Examples

- Plane-wave electronic structure calculations
  - Fourier space confined in a sphere of diameter d
  - Real space in a 2d^3 cube
  - Only transpose non-zero data to improve efficiency
    - d*d*2d; d*2d*2d
- CFD application using staggered mesh
  - Cell-centre variables and cell-interface variables different global sizes



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FFT Engines

- Distributed library performs data management only.
- Actual 1D FFT delegates to a third-party FFT library.
- Multiple third-party libraries supported.

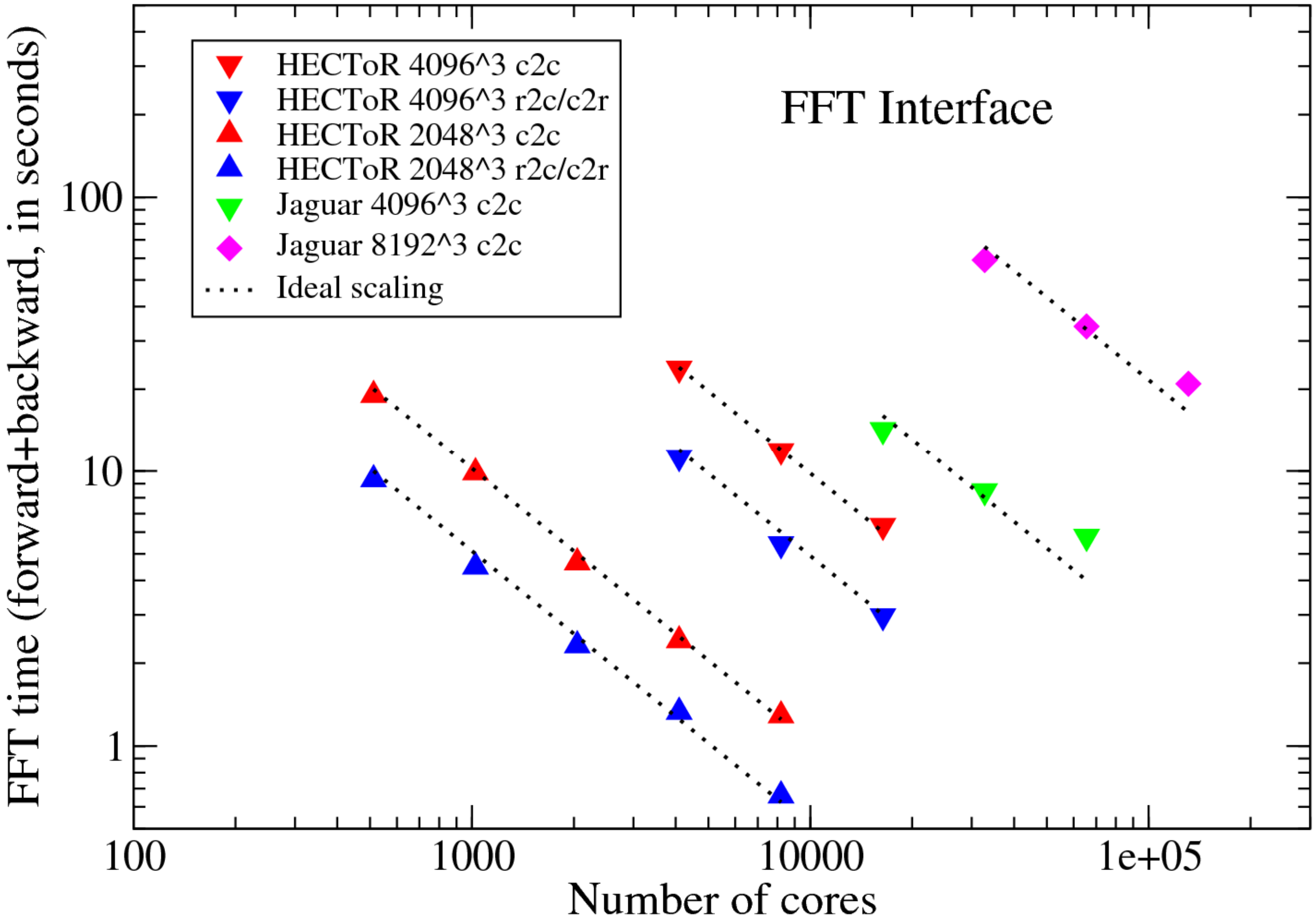
Library	Open-source	Hardware-tuned	Programming experience	Easy parallel coding
Generic (default)	Y	N	Slow but no dependency on external library	Y
FFTW 3.x	Y	Auto-tuning	Planning hard to use in parallel coding	N
ACML	N	For AMD	Limited r2c/c2r API	Y
fftpack	Y	N	Slow but used in many legacy applications	Y
MKL	N	For Intel	Flawed API design	Y
ESSL	N	For IBM	Limited transform lengths	N

FFT Library Performance

N^3	Serial FFTW		Distributed (FFTW engine)		
	Planning	Execution	16 cores	64 cores	256 cores
64^3	0.359	0.00509	0.00222	-	-
128^3	1.98	0.0525	0.0223	0.00576	0.00397
256^3	8.03	0.551	0.179	0.0505	0.0138
512^3	37.5	5.38	1.74	0.536	0.249
1024^3	-	-	-	4.59	1.27
2048^3	-	-	-	-	17.9

- Problem size increased by 8.
- Serial FFTW's execution time increased by ~10.
- Distributed FFT follows serial trend.

FFT Library Scaling



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Distributed Poisson Solver

- Fourier-based matrix decomposition method
  - Idea:
    - Finite difference discretisation of 3D Poisson results in matrix with 7 diagonal lines
    - Applying FFT in one dimension $\rightarrow$ 2D pentadiagonal systems
    - Applying FFT in a second dimension $\rightarrow$ 1D tridiagonal systems
  - FFT in X $\rightarrow$ FFT in Y $\rightarrow$ tridiagonal solver in Z $\rightarrow$ Inverse FFT in Y $\rightarrow$ Inverse FFT in X
  - Non-periodic data sets
    - Discrete sine/cosine/quarter-wave transforms
    - Passed to standard FFT library with pre- & post-processing
  - Library code available: FISHPACK, FFTPACK
  - Fit in current framework for parallelisation

Distributed Poisson Solver (2)

- Fourier-based spectral method
  - Algorithm
    - Pre-processing in physical space
    - 3D forward FFT
    - Pre-processing in spectral space
    - Solve Poisson by division of modified wave numbers
    - Post-processing in spectral space
    - 3D inverse FFT
    - Post-processing in physical space
  - Standard 3D FFT in use even with non-periodic data sets
  - Pre- and post-processing can be **local** (done in any pencil orientation) or **global** (data transpositions required)

Poisson Solver Performance

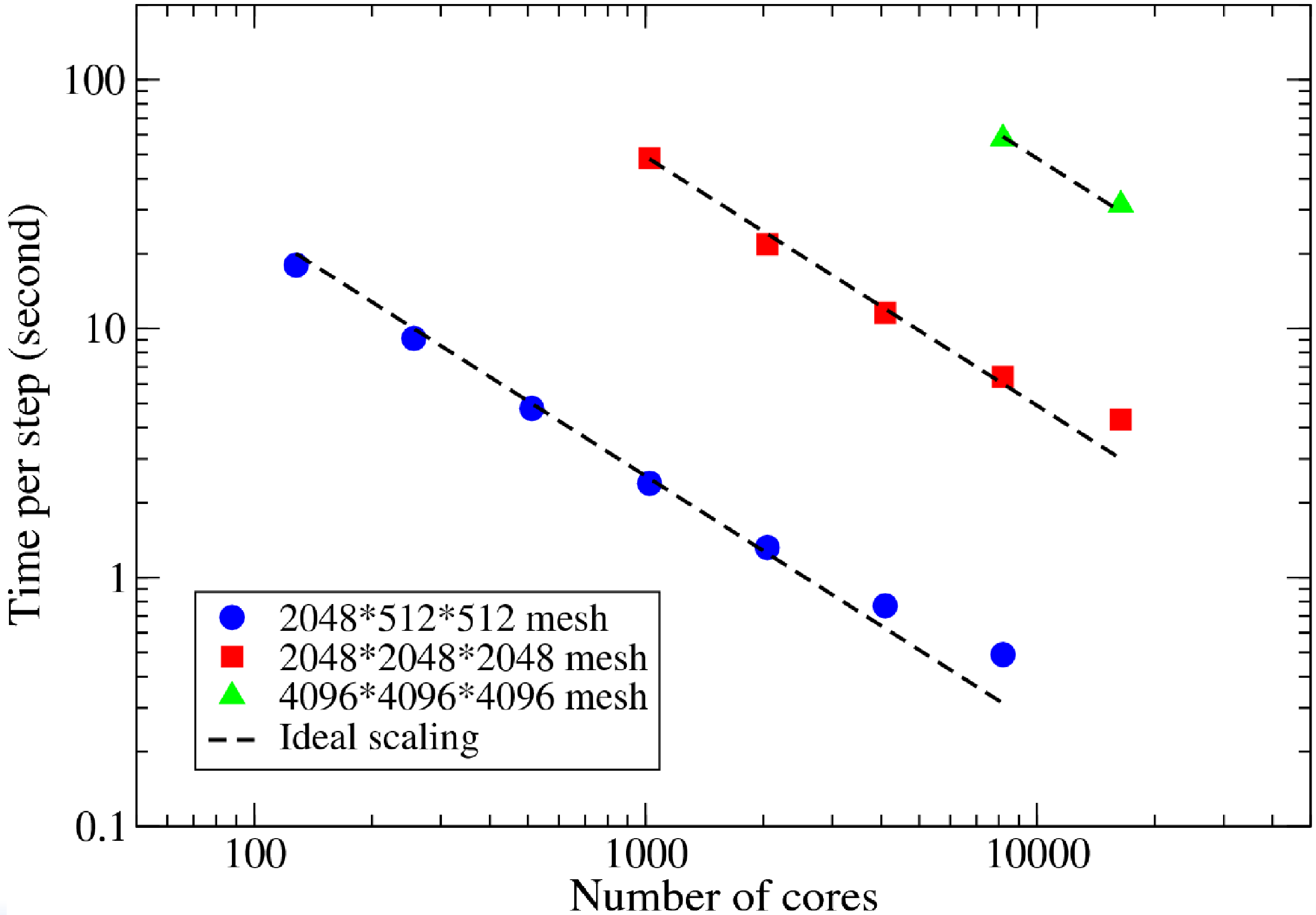
Boundary Condition	Global Transpositions	1024^3 case on 128 cores	2048^3 case on 1024 cores	4096^3 case on 8192 cores
000	FFT only	4.81	6.26	7.59
100	FFT + 8	7.38	10.38	14.41
010	FFT + 6	6.81	8.86	12.63
110	FFT + 12	8.23	11.56	16.31
111		8.41	11.67	16.48

- Boundary conditions:
  - 0 – periodic
  - 1 – homogeneous Neumann (symmetric)
- FFT (forward + inverse) contain 4 global transpositions
- Computationally dominant algorithm even with extra communications

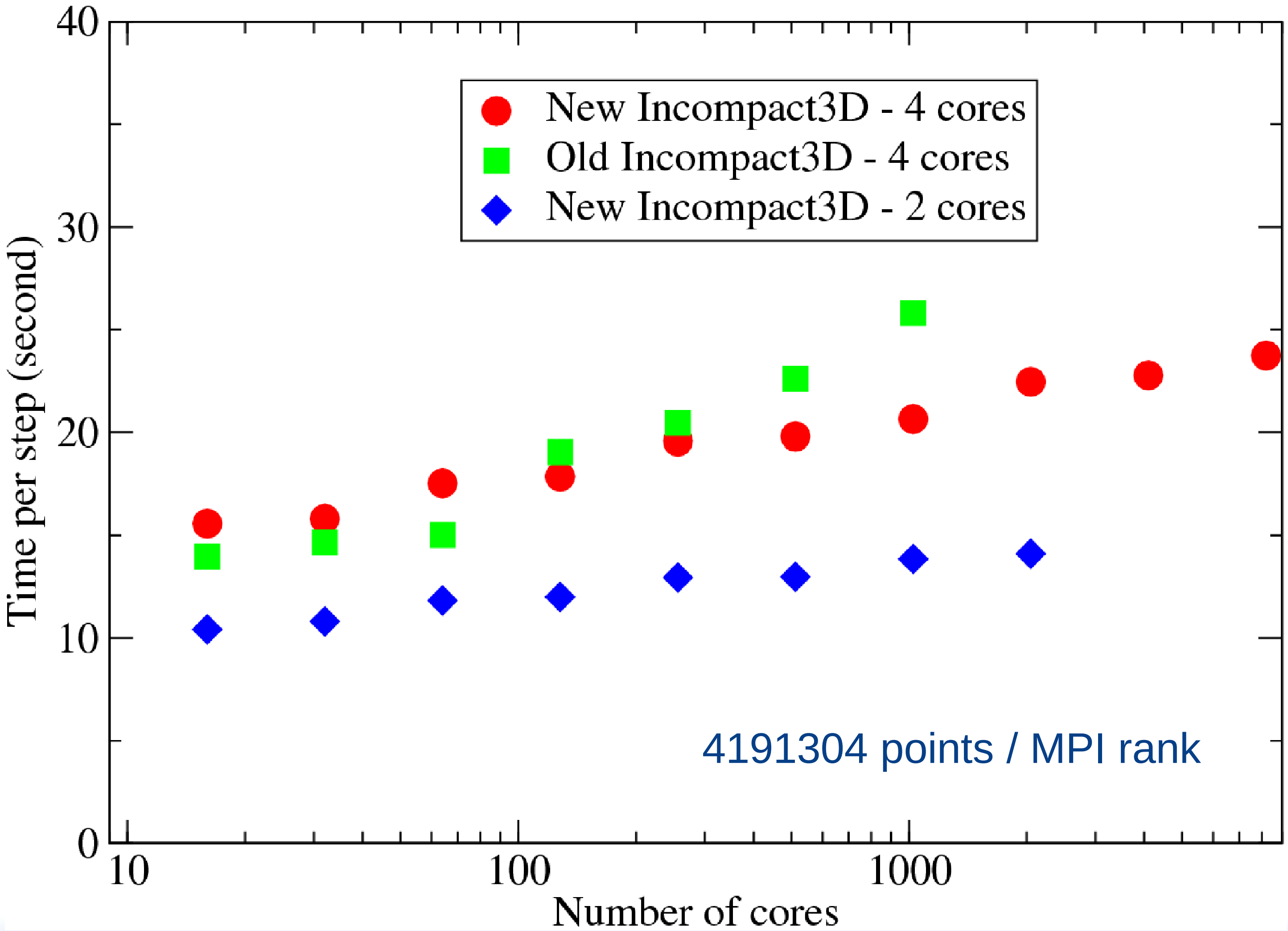
Putting all together

- CFD code Incompact3D uses
  - Explicit data transpositions for its finite difference part when
    - Computing spatial derivatives
    - Doing spatial interpolations
    - Doing spatial filtering
  - A modified version of the Poisson solver for pressure Poisson problem
    - Indirectly using the FFT library
  - In total up to 66 transposition calls per time step
  - An I/O library, also built using the decomposition data

Incompact3D Strong Scaling on HECToR



Incompact3D Weak Scaling on HECToR



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Summary

- Highly scalable and user-friendly 2D decomposition library and distributed FFT library developed.
- Framework for parallelising other algorithms as long as they are
  - Based on 3D Cartesian data structures
  - Operating on direction by direction basis
- Very successful application in Incompact3D

- Source code available upon request
  - Email ning.li@nag.co.uk
  - Collaboration opportunities?

Questions?

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