Large-scale Applications made Fault-tolerant using the Sparse Grid Combination Technique

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(slides available from http://cs.anu.edu.au/~Peter.Strazdins/seminars)

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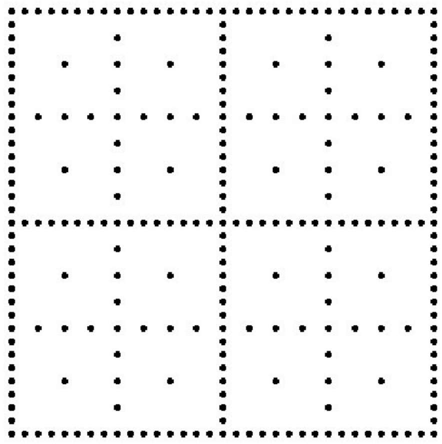
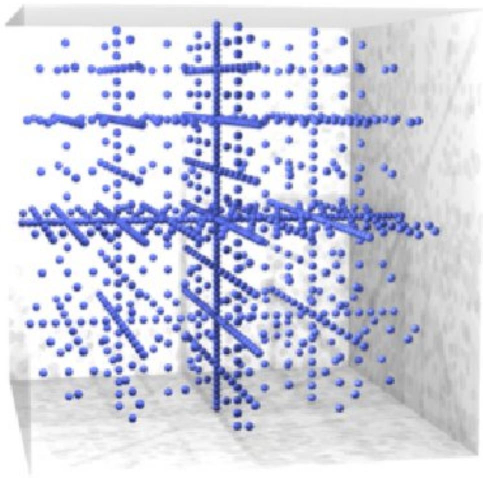
1 Talk Overview

- background: solving PDEs via sparse grids with the combination technique, hierarchical surplus representation
- parallel sparse grid combination technique (SGCT) algorithms
  - mappings for the block distribution in d-dimensional space
  - direct SGCT algorithm: idea, components, overall
  - hierarchical surplus algorithm: forming surpluses, coalescing surpluses, direct SGCT extensions
  - limitations and extensions
- analysis & experimental results (on Raijin cluster, NCI National Facility)
- making real-world applications fault tolerant using the SGCT
  - general methodology
  - process recovery using ULFM MPI
  - GENE gyrokinetic plasma, Taxila Lattice Boltzmann method, Solid Fuel Ignition
- conclusions and future work

2 Background: Sparse Grids

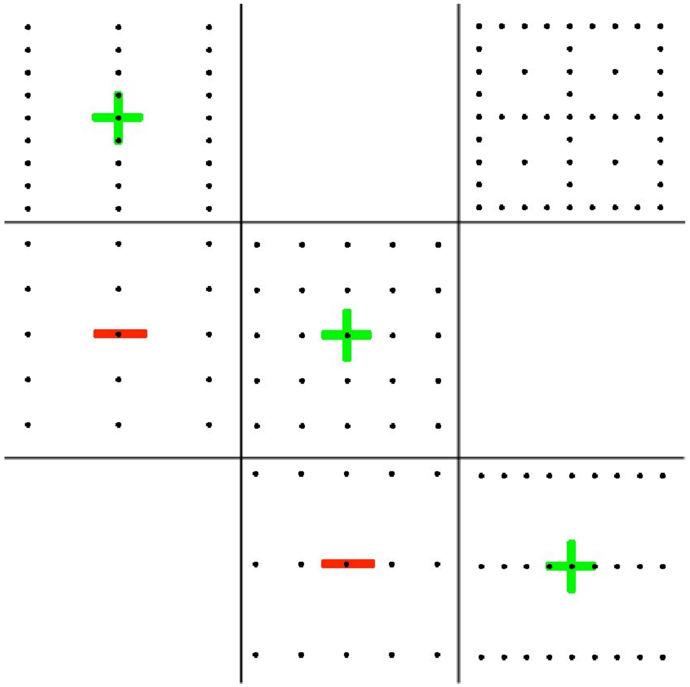
- introduced by Zenger (1991)
- for (regular) grids of dimension d having uniform resolution n in all dimensions, the number of grid points is n^d
  - known as the *curse of dimensionality*
- a sparse grid provides fine-scale resolution
- can be constructed from regular sub-grids that are fine-scale in some dimensions and coarse in others
- has been proven successful for a variety of different problems:
  - good accuracy for given effort (over single higher resolution grid)
  - various options for fault-tolerance!

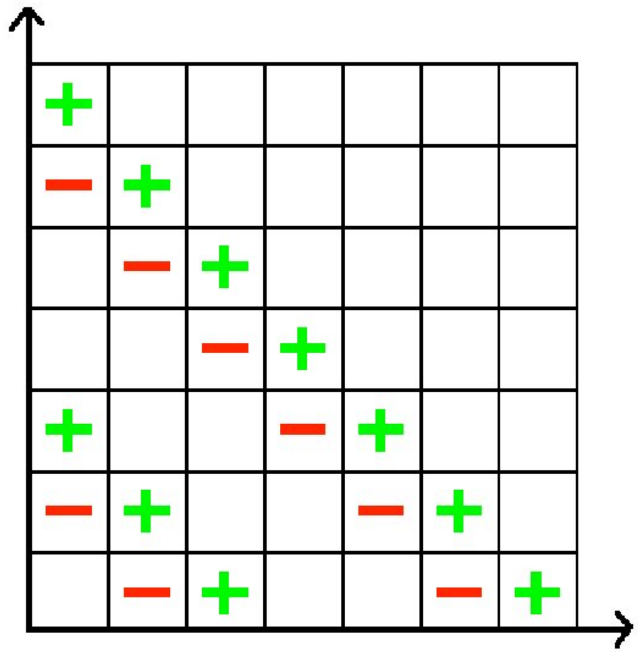




3 Background: Combination Technique for Sparse Grids

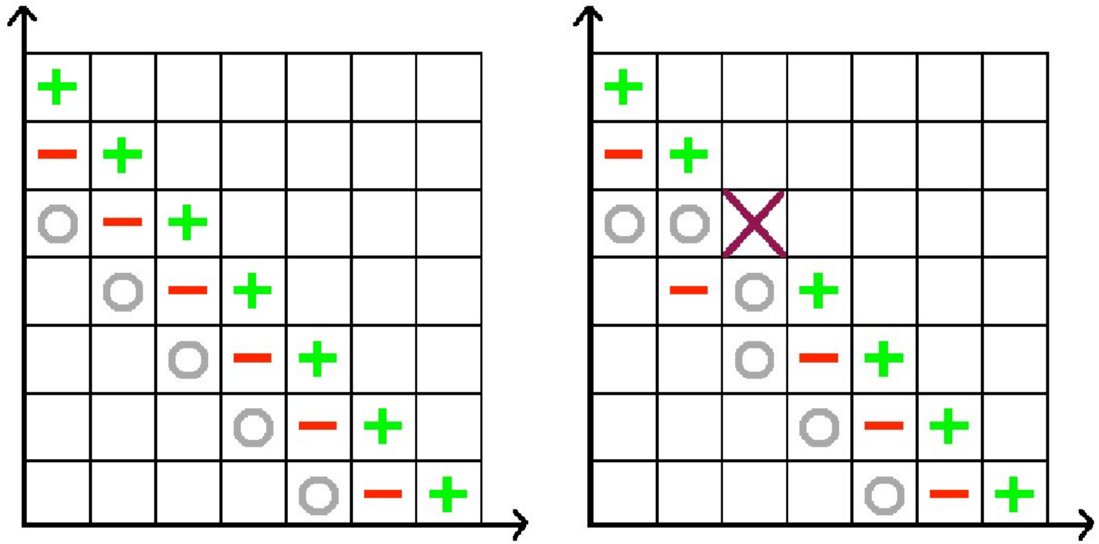
- computations over sparse grids may be approximated by being solved over the corresponding set of regular sub-grids
  - overall solution is from 'combining' sub-solutions via an inclusion-exclusion principle (complexity is still $O(n \lg(n)^{d-1})$)
- for 2D at 'level' $l = 3$, combine grids $(3,1)$, $(2,2)$ $(1,3)$ minus $(2,1)$, $(1,2)$ onto (sparse) grid $(3,3)$ (interpolation is required)





4 Robust Combination Techniques

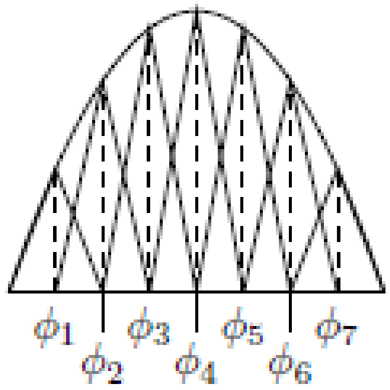
- uses extra set of smaller sub-grids with $||i||_1 = m - d$ (now $m \geq d$)
  - the redundancy from this is $< 1/(2(2^d - 1))$
- for a single failure on a sub-grid, can find a new combination formula with an inclusion/exclusion principle avoiding the failed sub-grid
- works for many cases of multiple failures (using a 4th set covers all)
- a failed sub-grid can be recovered from its projection on the combined sparse grid

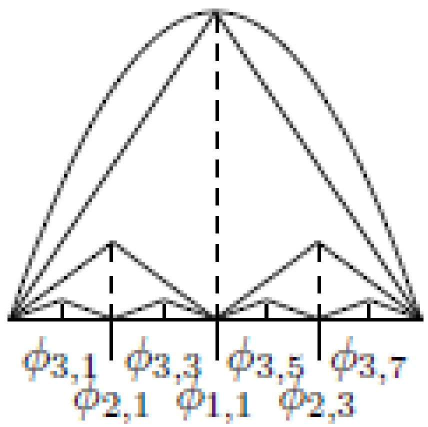


5 Background: Hierarchical Surplus Representation of Grids

- normally use a nodal representation: the value at point x_k is $v_k = f(x_k)$
- we can also use a hierarchical representation: the value at $x_{l,k}$ is the difference between that at $x_{l,k}$ and its hierarchical neighbours (l denotes the 'level')

$$v_{l,k} = \begin{cases} f(x_{l,k}) - \frac{1}{2}\left(\begin{array}{l} f(x_{l-1,(k-1)/2}) \\ +f(x_{l-1,(k+1)/2}) \end{array} \right) & \text{for } l > 0 \\ f(x_{l,k}) & \text{for } l = 0 \end{cases}$$





- we can perform the combination algorithm on each of the component grid's common hierarchical surpluses (a grid of index (i, j) has $(i+1)(j+1)$ surpluses)
  - √ this reduces communication (surpluses corresp. to the upper diagonal are unique) and avoids interpolation

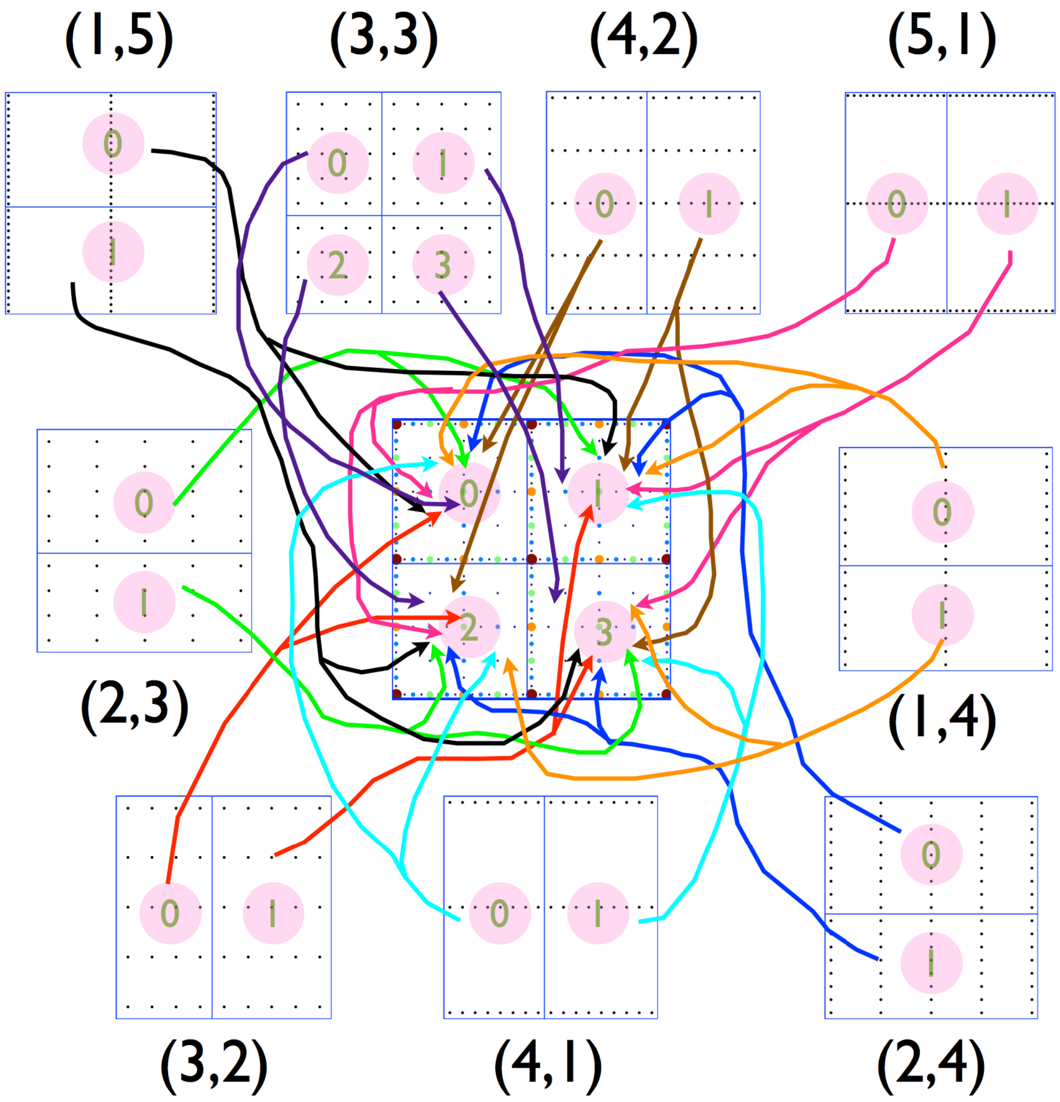
6 Background: Hierarchical Surplus Formation

- on a component grid (G_i), each element will correspond to a hierarchical surplus of index j, where $j \leq i$
- e.g. for $i = (3, 3)$

00	30	20	30	10	30	20	30	00
03	33	23	33	13	33	23	33	03
02	32	22	32	12	32	22	32	02
03	33	23	33	13	33	23	33	03
01	31	21	31	11	31	21	31	01
03	33	23	33	13	33	23	33	03
02	32	22	32	12	32	22	32	02
03	33	23	33	13	33	23	33	03
00	30	20	30	10	30	20	30	00

- the hierarchization process occurs in-place, with the surpluses computed from the initial grid values
- note that the size of surplus of index j is 2^j – independent of G_i
- hierarchical surpluses contain common information across different component grids

7 Direct SGCT Algorithm: the Gather-Scatter Idea



- evolve independent simulations over set of component grids, solution is a d-dimensional field (here d=2)
- each grid is distributed over a process grid (here these are 2×2, 2×1 or 1×2)
- gather: after a simulated time T is reached, combine fields on a sparse grid (here level 5, or index $(5, 5)$)
- scatter: sample (the more accurate) combined field and redistribute back to the component grids

8 Mappings for the d-dimensional Block Distribution

- can be succinctly expressed in terms of d-dimensional vector arithmetic
  - for $M = (M_x, M_y), N = (N_x, N_y) \in \mathbb{N}^d$, and $a \in \mathbb{N}$,
    $M \le N \equiv (M_x \le N_x) \wedge (M_y \le N_y)$; $a \le N \equiv (a \le N_x) \wedge (a \le N_y)$
    $M * N \equiv (M_x * N_x, M_y * N_y)$; $a * N \equiv (a * N_x, a * N_y)$
    $\Pi(N) = N_x * N_y$
- we have the following mappings for the block-distribution of a global length $N \in \mathbb{N}^d$ over a process grid $P \in \mathbb{N}^d$,

  for a process of id $p \in \mathbb{N}^d$, $0 \le p < P$,

  and for a global index $\hat{N} \in \mathbb{N}^d$, $0 \le \hat{N} < N$:

  $l(N, p, P) = n + (p == P - 1) * (N\%P)$: local length of N at p
  $g_0(N, p, P) = p * n$: global index of local index 0 at p
  $p(\hat{N}, N, P) = \min(\hat{N}/n, P - 1)$: id of process holding global index $\hat{N}$
  $o(\hat{N}, N, P) = \hat{N}\,\%\,n$: local offset within this process corresponding to $\hat{N}$

  where $n = N/P$

9 Direct SGCT Algorithm: Gather Stage

- for component grid of size N on process grid P; sparse grid is of size N' on process grid P' ($r = (N'-1)/(N-1)$): sending part is:

$\hat{N}' = rg_0(N, p, P);$ // scaled global starting index on P
$p' = p(\hat{N}', N', P');\ \hat{o}' = o(\hat{N}, N', P');$ // process id & local offset on P' . . .
// . . . for 1st message

i=0; $n = l(N, p, P);$
while $i_x < n_x$
  while $i_y < n_y$
    $o' = \hat{o}' * (i{=}{=}0);$ // local offset @ p'
    $n' = l(N', p', P') - o';$ // local size @ p'
    $dn = \min(n'/r, n - i);$ // local size here
    send local points $i : i + dn$ of u to p'; // extra points for interpolation
    i_y+=$dn_y;\ p'_y$++;
  i_x+=$dn_x;\ p'_x$++;

- receiving part is similar, except each component grids' message is performed serially & received points are interpolated into the sparse grid

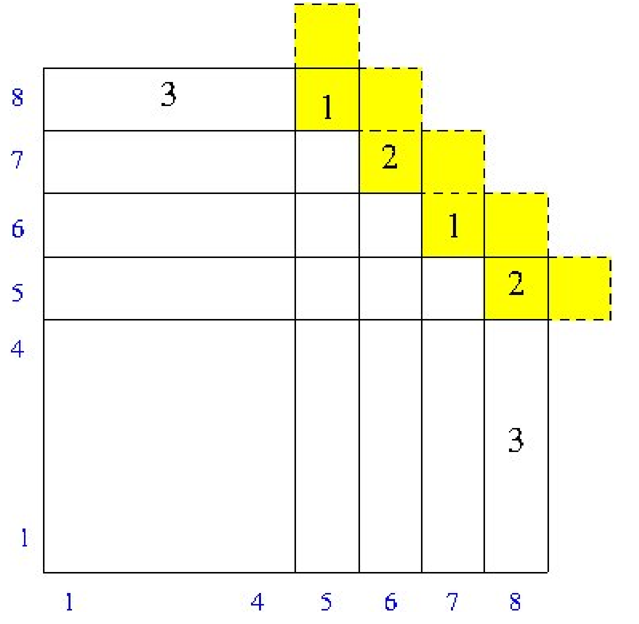
10 Direct SGCT Algorithm

- scatter stage, similar to gather (in reverse)
  - send stage on sparse grids' process grid *down-samples* respective points for each component grid
- for fault tolerance, a 3rd (smaller) diagonal of component grids is utilized
  - if a process on a component grid fails, a revised set of combination coefficients are supplied to the SGCT (with 0 for the failed grid)
  - the algorithm (and implementation) are otherwise unaffected
- only limitation in terms of process grid size of algorithm is that P' must be a power of 2
  - can be overcome if we send extra points to left for interpolation
- current implementation supports $d \leq 3$
  - main complexity for extending to larger d is in enumerating the component grids and the interpolation routine
  - can deal with $d' > 3$ dim. fields if only d dims. are used for the SGCT
  - the gather is performed on a (partial) sparse grid data structure

11 Hierarchical Surplus-Based SGCT Algorithm

Overall algorithm:

1. hierarchize each component grid, min-place (independently)
   - involves $\Pi(\lg_2 N)$ send-receive stages
2. apply the (direct) SGCT over each hierarchical sub-space common to > 1 process grids
   - in each, only the process grids involved need participate
   - note that interpolation is *not* required as each surplus is the same size on each grid
3. un-hierarchize the surpluses to recover the original grids

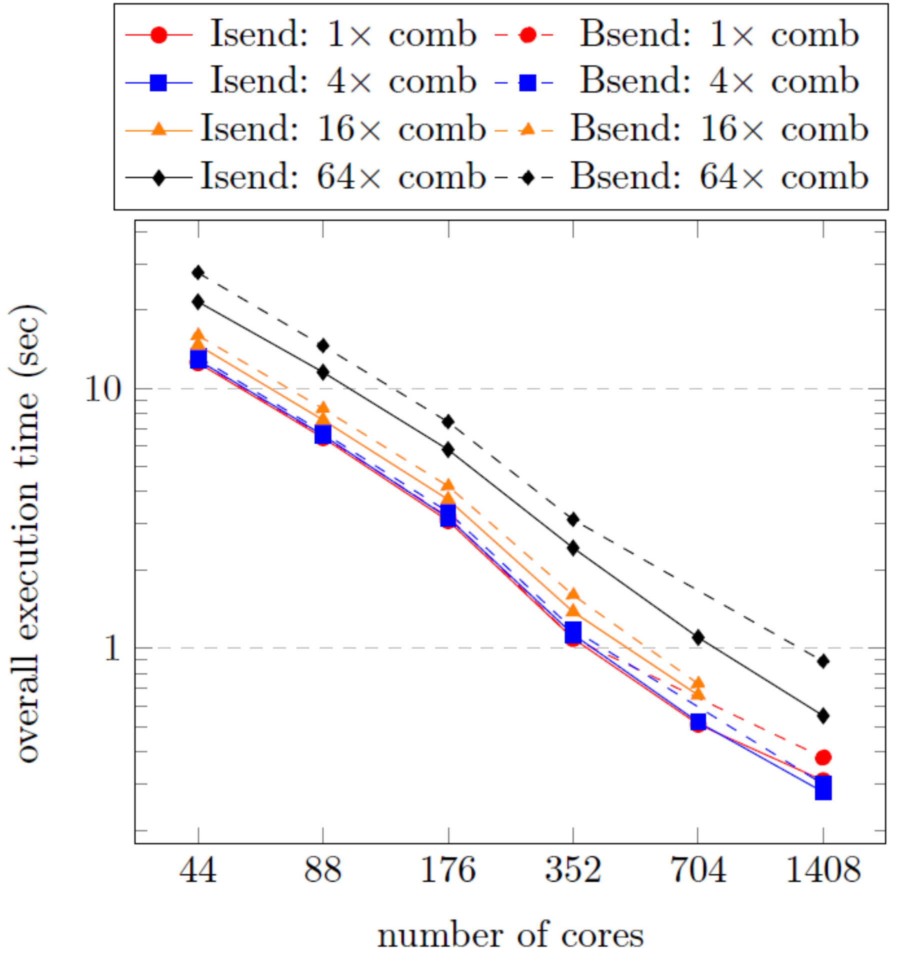


A 2D $l = 5$ SGCT on a sparse grid of index $(9, 9)$.
Indices of component grids are in yellow.
Can coalesce SGCT over sub-spaces to reduce overheads.

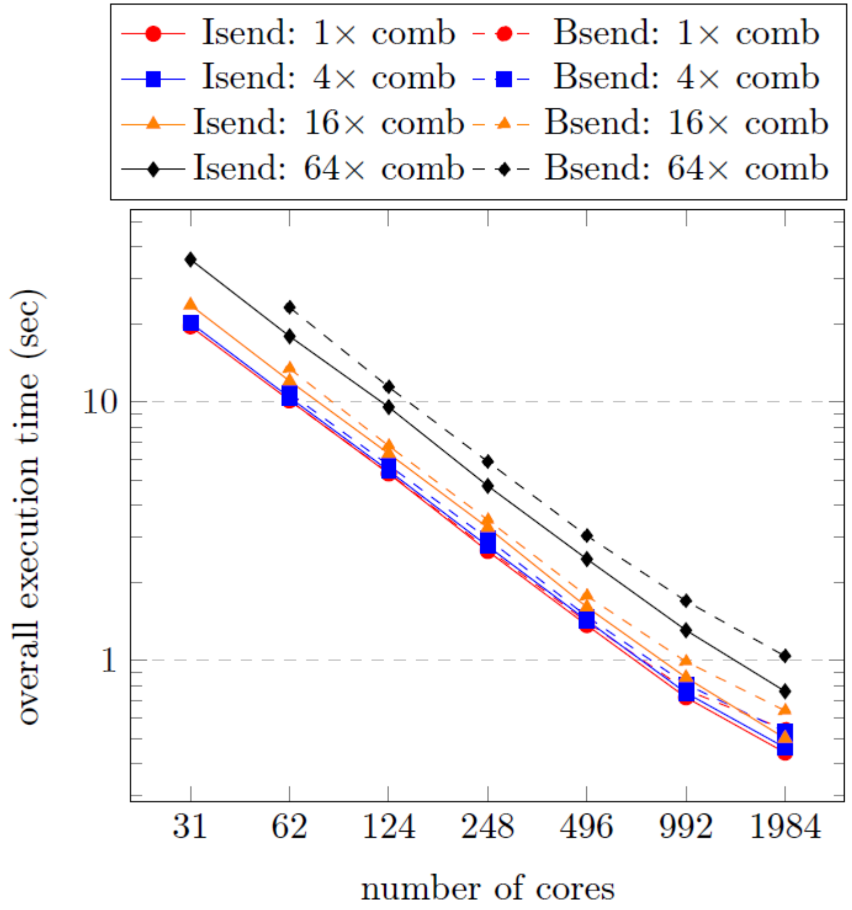
12 Analysis

- typical operating conditions of the SGCT:
  - the sparse grid's process grid P' comprises of a subset of processes from the process grids of the components (P_i)
  - assume P_i, P' are powers of 2 (required for hierarchical algorithm)
  - each sub-grid on a lower diagonal has half the processes as that above
- let $g = g(d, l) = O(l^{d-1})$ be the number of sub-grids involved, m denote the number of data points per process
- direct SGCT, each process in P' will receive $< 2m$ points, each process in each P_i sends and receives $\Pi(P'/P_i) \leq g$ messages
  - total cost is then $t^{\mathrm{d}} \leq 2g\alpha + 3m\beta$
  - should be efficient for large m, but not for large g
- hierarchical SGCT avoids communication of $\frac{1}{2^d}$ of the surpluses
  - will have more startups even if coalesced, partially offset by a ≈30% lower average effective value of g
  - average degree of $||$ization $\approx 2/3$, but a load imbalance factor of $\approx 2^d$

13 Results: SGCT Advection Performance



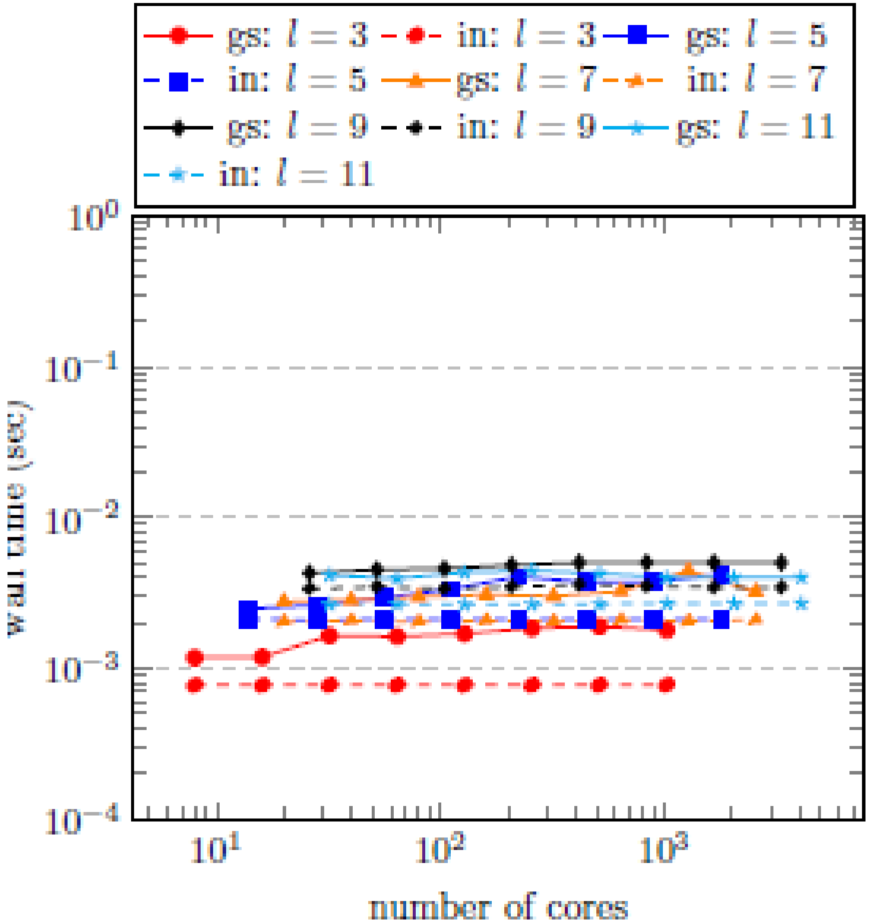
(a) 2D problem with $l = 4$ and a $2^{13} \times 2^{13}$ (sparse) grid, 1024 timesteps.

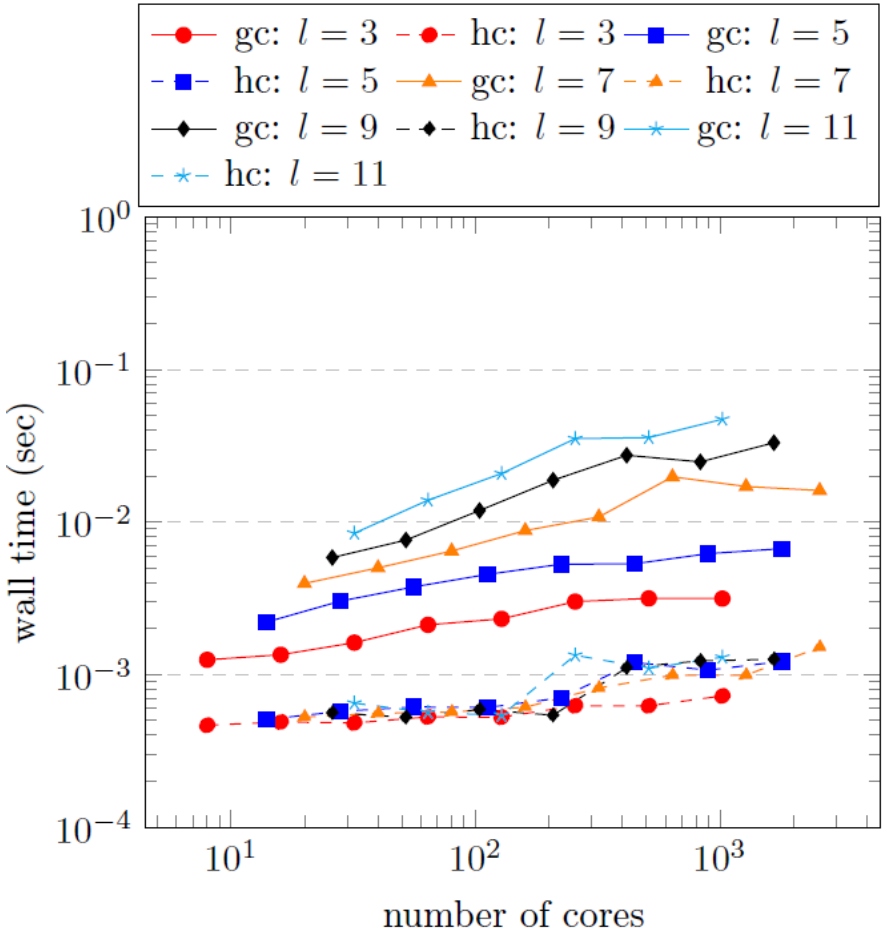


(b) 3D problem with $l = 3$ and $2^9 \times 2^9 \times 2^8$ grid, 1024 timesteps.

14 Results: 2D SGCT Algorithm Performance

Weak Scaling with $m = 2^{14}$ points per process for 2D SGCT performance (*after* a warmup run) with SGCT level l: direct (left) vs hierarchical





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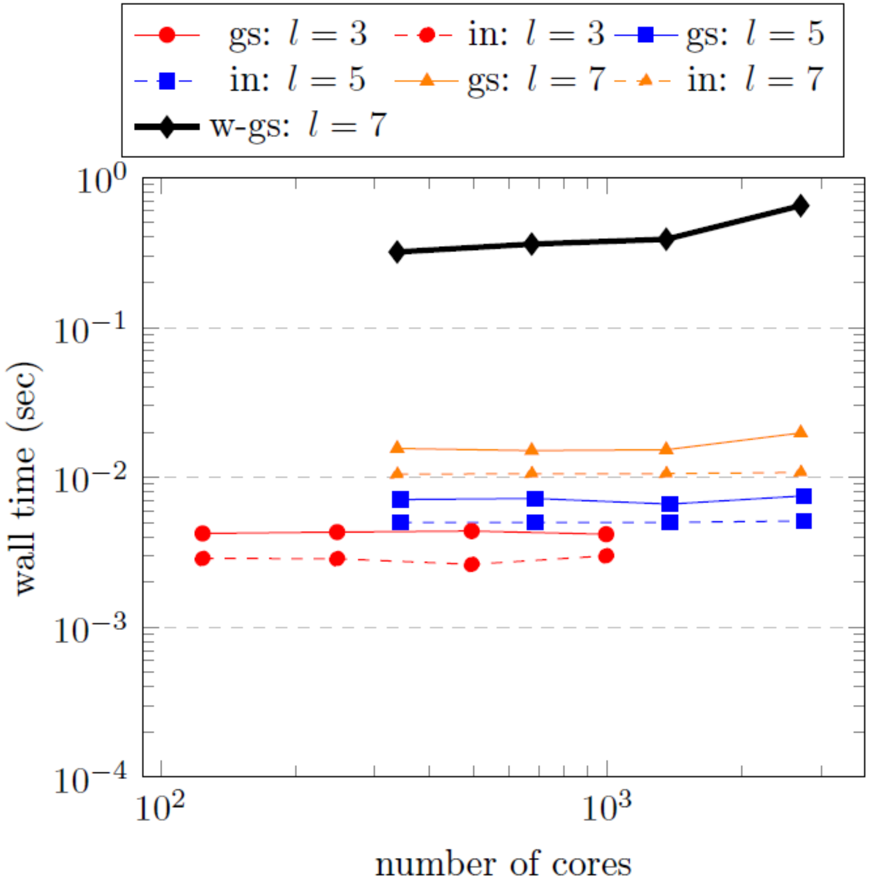
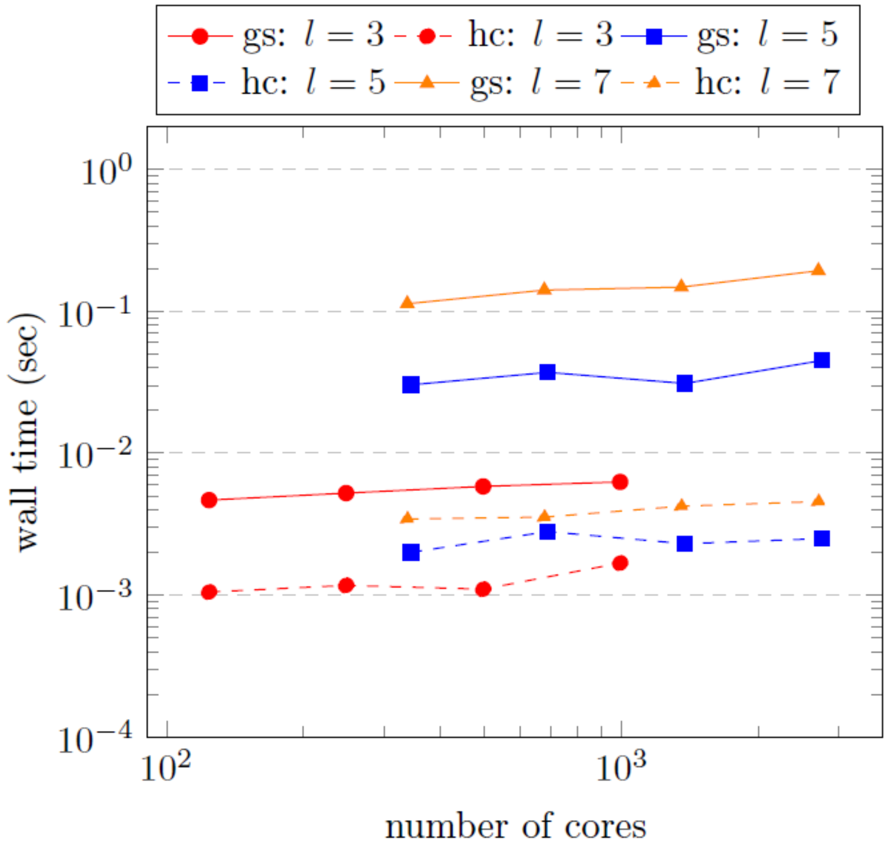
15 Results: 3D SGCT Algorithm Performance

Weak scaling with $m = 2^{14}$ points per process for 3D SGCT performance (*after* a warmup run) with SGCT level l:

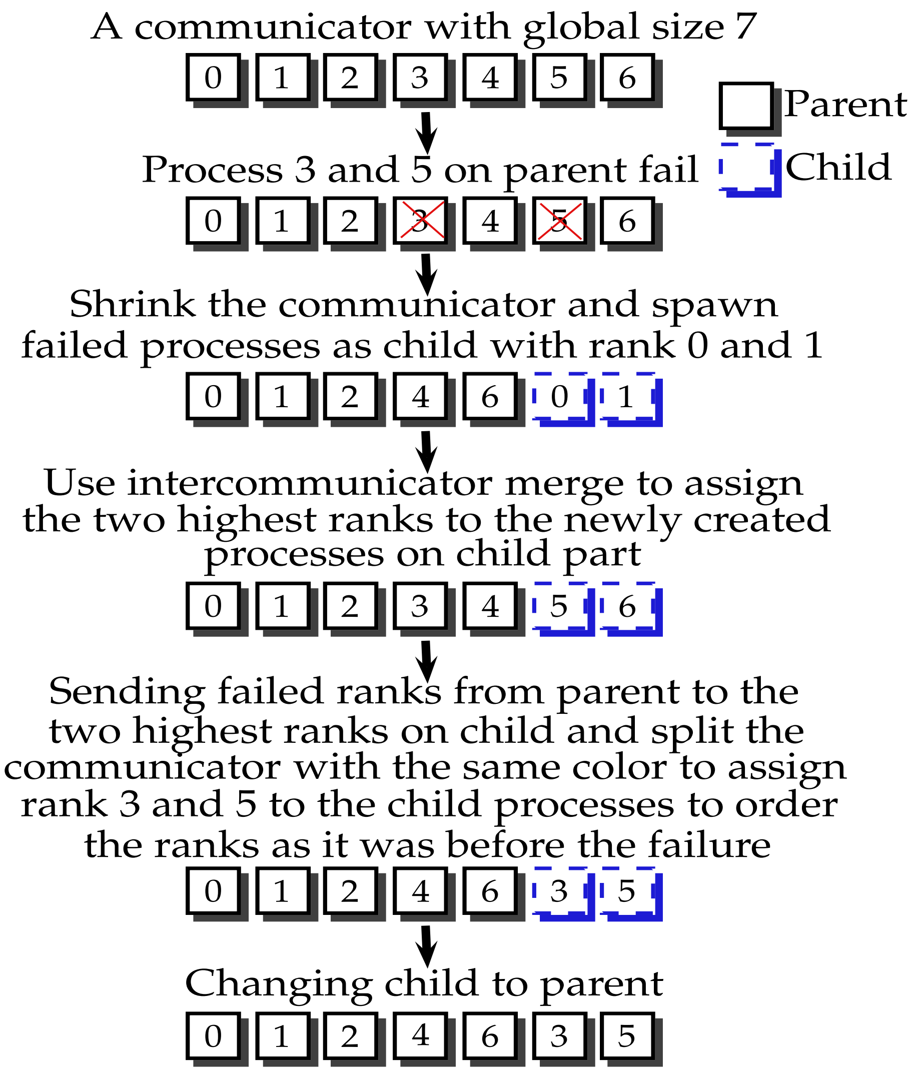


(a) direct algorithm



(b) hierarchical algorithm

16 Fault Recovery Procedure: Detect Failed Processes



- can detect failed processes in ULFM MPI as follows:
  - attach an error handler ensuring failures get acknowledged on (original) communicator `comm`
  - call `MPI_Barrier(comm)`; if fails:
  - revoke it via `MPI_Comm_revoke(comm)` and create shrunken communicator via `OMPI_Comm_shrink(comm, &scomm)`
  - use `MPI_Group_difference(..., &fg)` to make a globally consistent list of failed processes

17 Fault Recovery Procedure: Process and Data

- process recovery in ULFM MPI:
  - use `MPI_Group_translate_ranks(fg, ..., comm, ...)` to re-rank remaining processes
  - spawn required number of failed processes via `MPI_Comm_spawn_multiple()`
    - these are called *child processes* and have own communicator
  - use `MPI_Intercomm_merge()` to merge child's comm. with parent's with `MPI_Comm_split()` to order the ranks
  - finally, `OMP_Comm_agree()` used to synchronize child and parent processes
- data recovery using the SGCT:

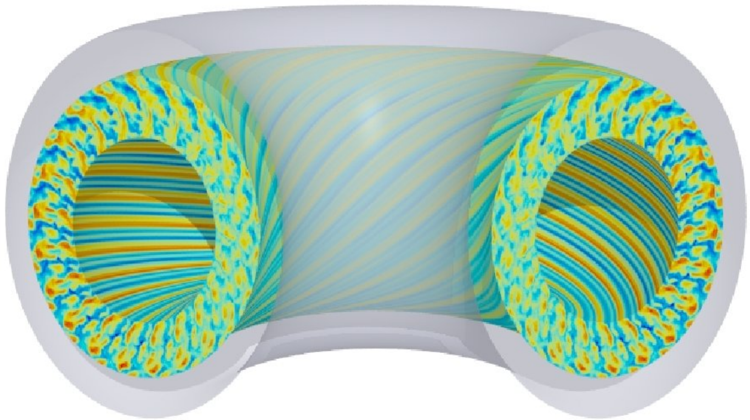
  must be done on whole of grid where a process has failed (data on non-failed process will be out-of-date)
  - identify lost grids; assign combination coefficient of 0 (do not participate in gather stage of SGCT)
  - receive down-sample of combined grid on the scatter stage

18 Methodology for Integrating the SGCT into an Application

$G = \{G_i\}$: set of sub-grids;
$C = \{C_i\}$: set of sub-grid communicators created from W;
$g = \{g_i\}$: set of fields returned from the application computed on G;
$u = \{u_i\}$: corresponding set of sub-grid solutions;
u_I^c: combined solution of the SGCT;
for each $C_i \in C$ **do in parallel**
  $u_i \leftarrow$ **null**; `//makes runApplication() initialize` g_i
for each required combination **do**
  for each $C_i \in C$ **do in parallel**
    $g_i \leftarrow$ runApplication(u_i, G_i, C_i);
    $u_i \leftarrow g_i$; `//on their common points`
    updateBoundary(u_i, C_i);
  reconstructFaultyCommunicator(W); `//using ULFM MPI`
  $u_I^c \leftarrow$ gather(u, W); `//reconstructed grids don't participate`
  $u \leftarrow$ scatter(u_I^c, W);

19 The GENE Application

- GENE: Gyrokinetic Electromagnetic Numerical Experiment
  - plasma micro-turbulence code
  - multidimensional solver of Vlasov equation
  - fixed grid in five-dimensional phase space $(x_r, x_\perp, x_{||}, v_\perp, v_{||})$



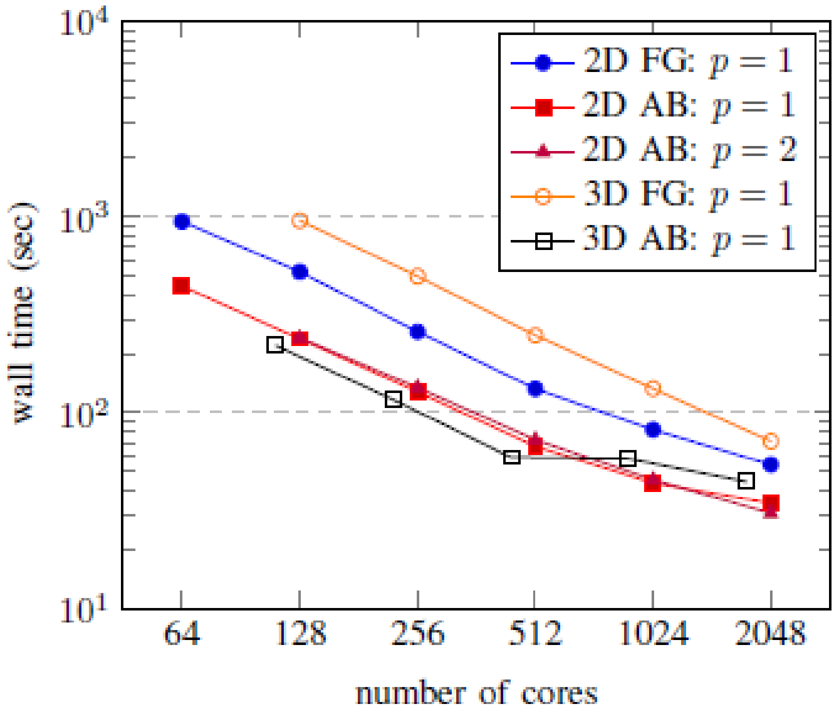
- computes gyroradius-scale fluctuations and transport coefficients
  - these fields are the main output of GENE
- hybrid MPI/OpenMP parallelization – high scalability to 2K cores
- dimensions are limited to powers of two
- sparse grid combination technique has yielded good results!
  - physical system is relatively homogeneous

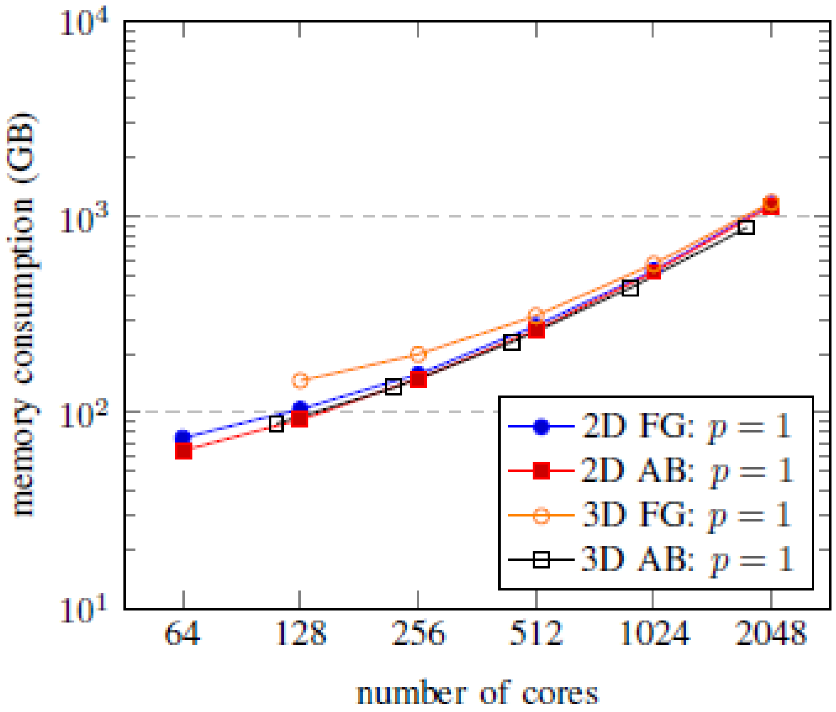
20 Incorporating the SGCT into GENE

- computes a density field `g_1`, stored in a double-precision array of dimensionality $(2, N_x, N_y, N_z, N_v, N_u, s)$, s is the number of 'species'
- the SGCT can be applied in any 2 or 3 contiguous dimensions

  e.g. for a 2D SGCT on N_v and N_u dimensions, we pass a block factor of $B = 2N_xN_yN_z$ to the SGCT algorithm, and iterate over s
- must pad dimensions of size 2^N to $2^N + 1$ for the SGCT: zero for v, u; for z, a 'shift' is required (using GENE routines)
- a parallelization of p over the non-SGCT dimensions is possible: perform p SGCT calculations in parallel
- a script creates different directories for each component grid to run in, and places an appropriately modified `parameters` file there
- `ISO_C_BINDING` & C wrappers to interface Fortran to C++ SGCT code
- small modifications to `rungene()` to pass down MPI communicator created by the SGCT constructor
- in `initial_value()`, code is added to pass `g_1` to the SGCT code

21 SGCT GENE Performance

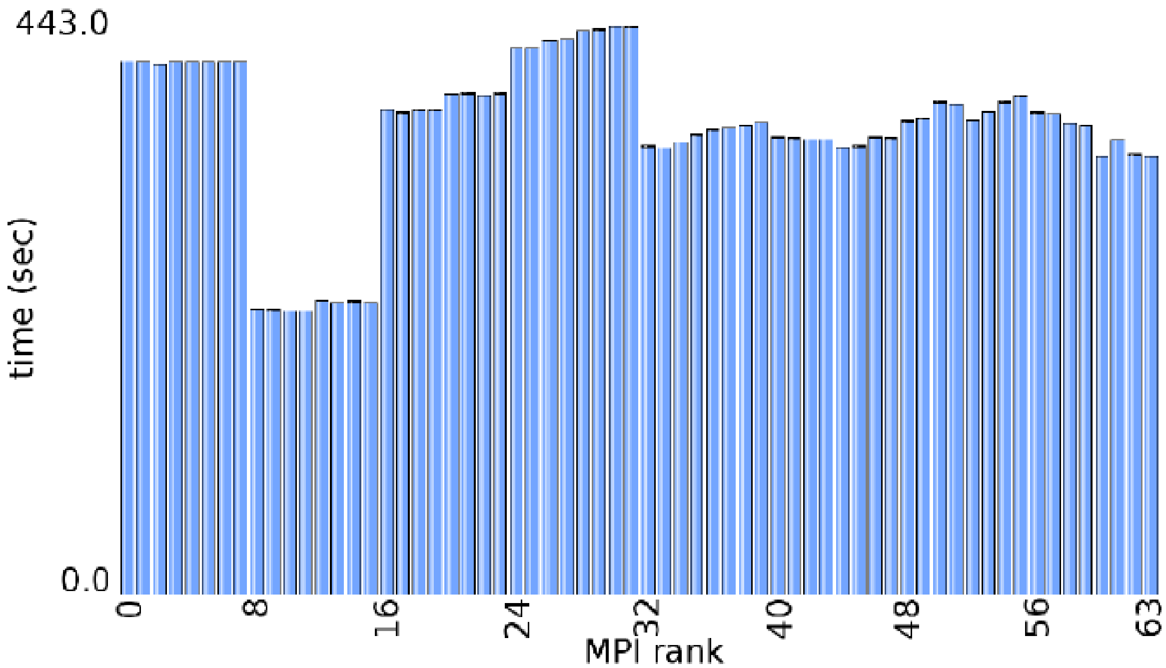




- used `2d_big_6` with an $l = 5$ 2D SGCT over $(N_v, N_u) = (2^8, 2^8)$ and $N_x = 64, N_y = 4, N_z = 16, s = 1$, and `3d_big_6` with an $l = 4$ 3D SGCT over $(N_z, N_v, N_u) = (2^6, 2^8, 2^8)$ and $N_x = 32, N_y = 4, s = 1$. Run for 100 timesteps.
- SGCT (AB) has less work & storage than the corresp. full grid (FG)

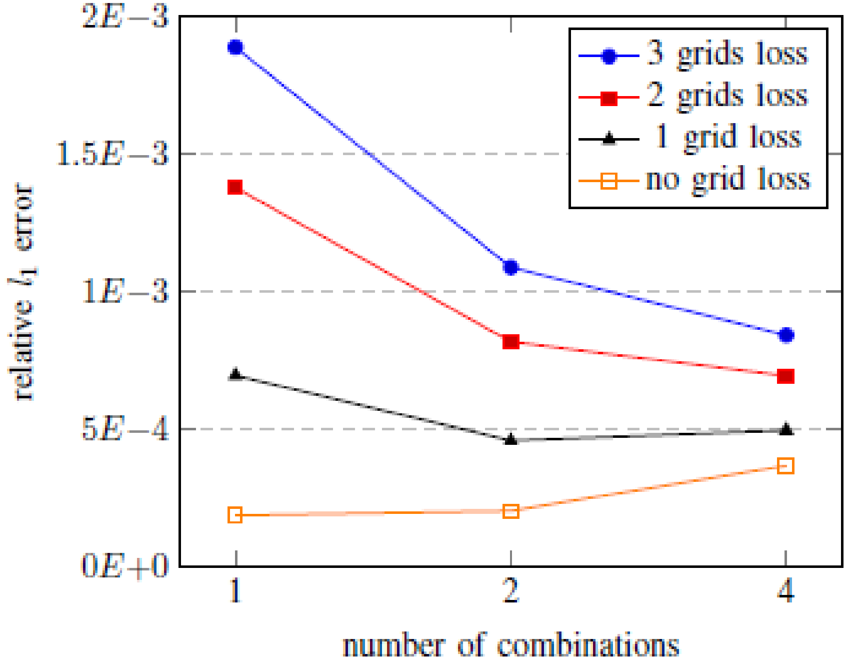
22 Load Balance for SGCT GENE

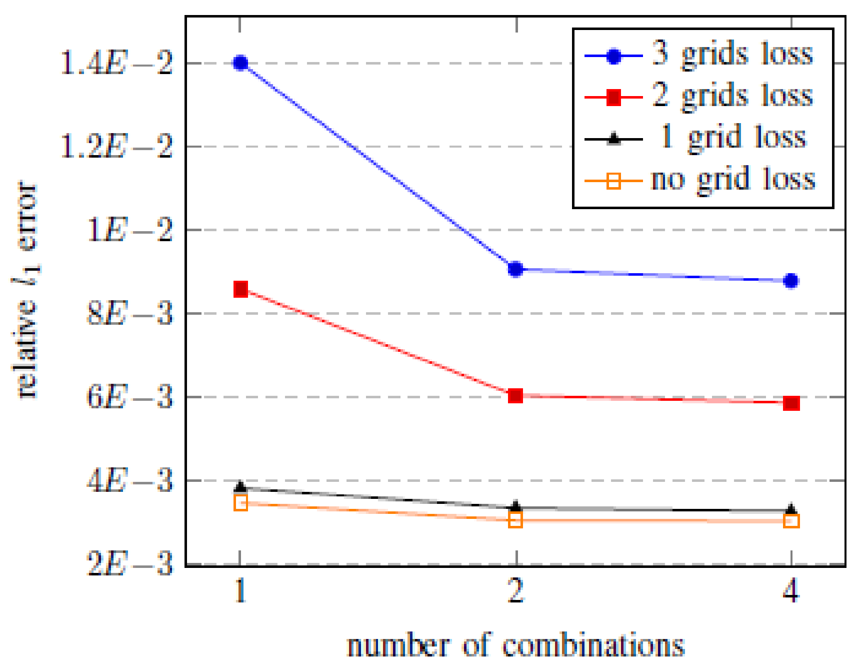
- general SGCT strategy to load balance across component grids
  - allocate p processes to uppermost diagonal grids, $\lceil \frac{p}{2} \rceil$ to next diag.
  - this, number of data points (hence work) per process should be equal
- however, data and process grid shape may affect computation and communication performance



- TAU profile for 2D problem with $p = 8$
- 3D problem & other apps were similar

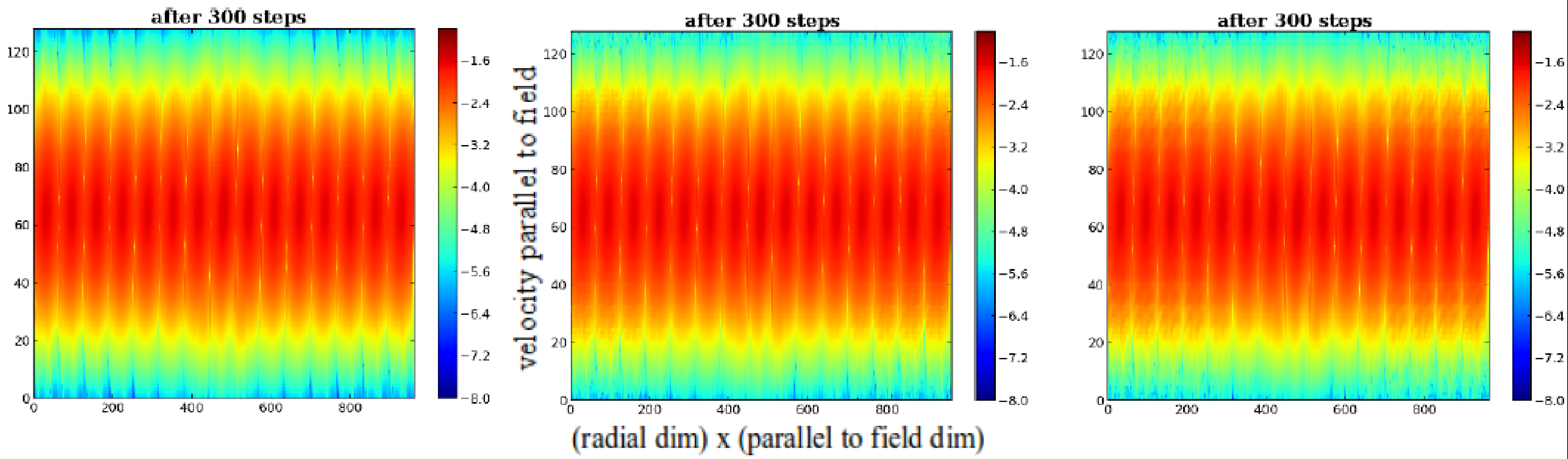
23 SGCT GENE Accuracy





- relative 1-norm error over full grid solution for 2D (left) and 3D (right)
- deemed ‘acceptable’
- multiple applications of the SGCT can reduce the error

24 SGCT GENE Accuracy - Visualization



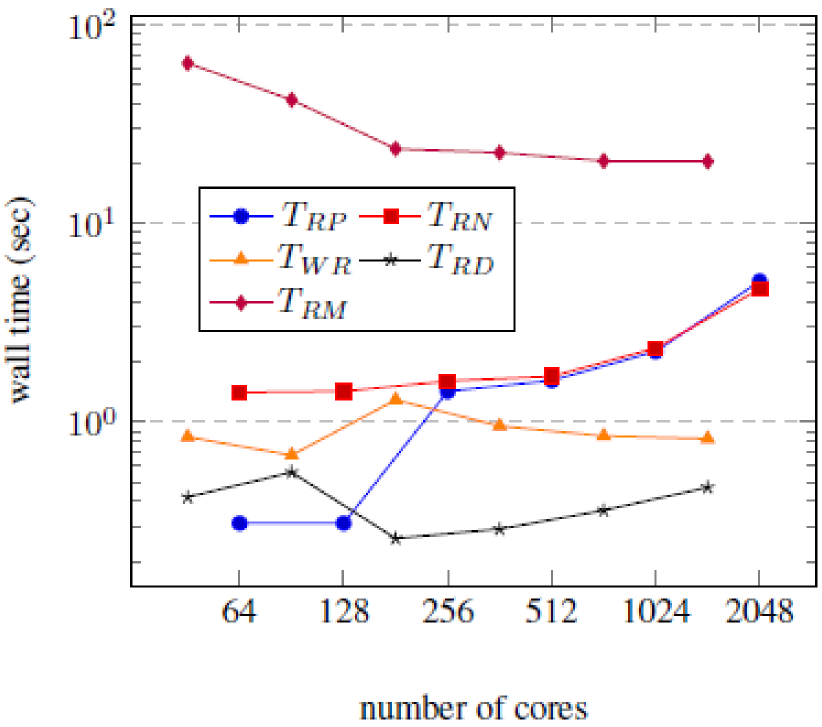
full grid field no failure

combined grid field no failure (relative l_1 error 5.0%)

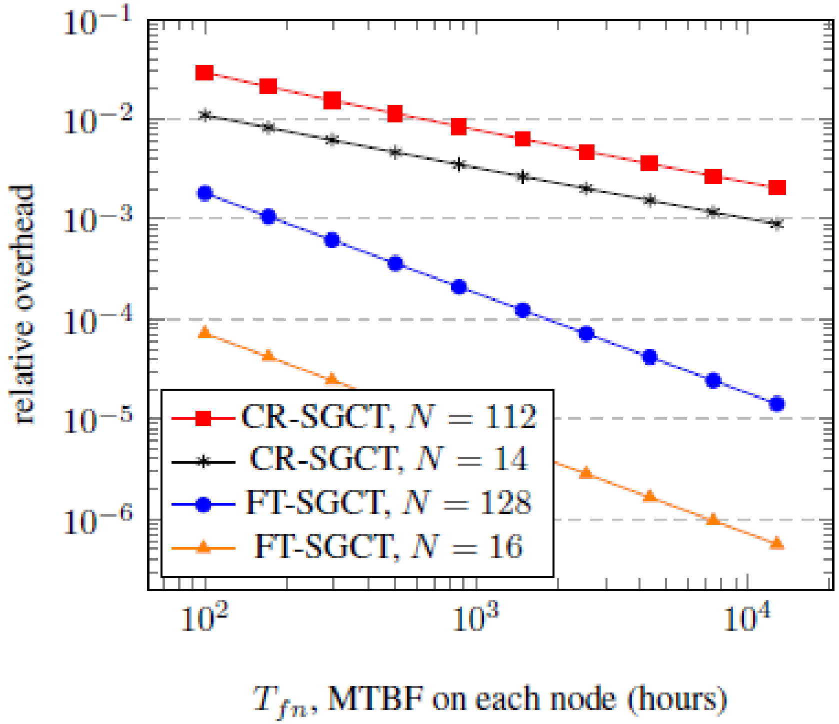
combined grid field 3 grids lost (relative l_1 error 6.22%)

- little discernible difference with or without faults

25 SGCT GENE Fault Recovery



(a) recovery overhead of a single occurrence of failure for shorter computation



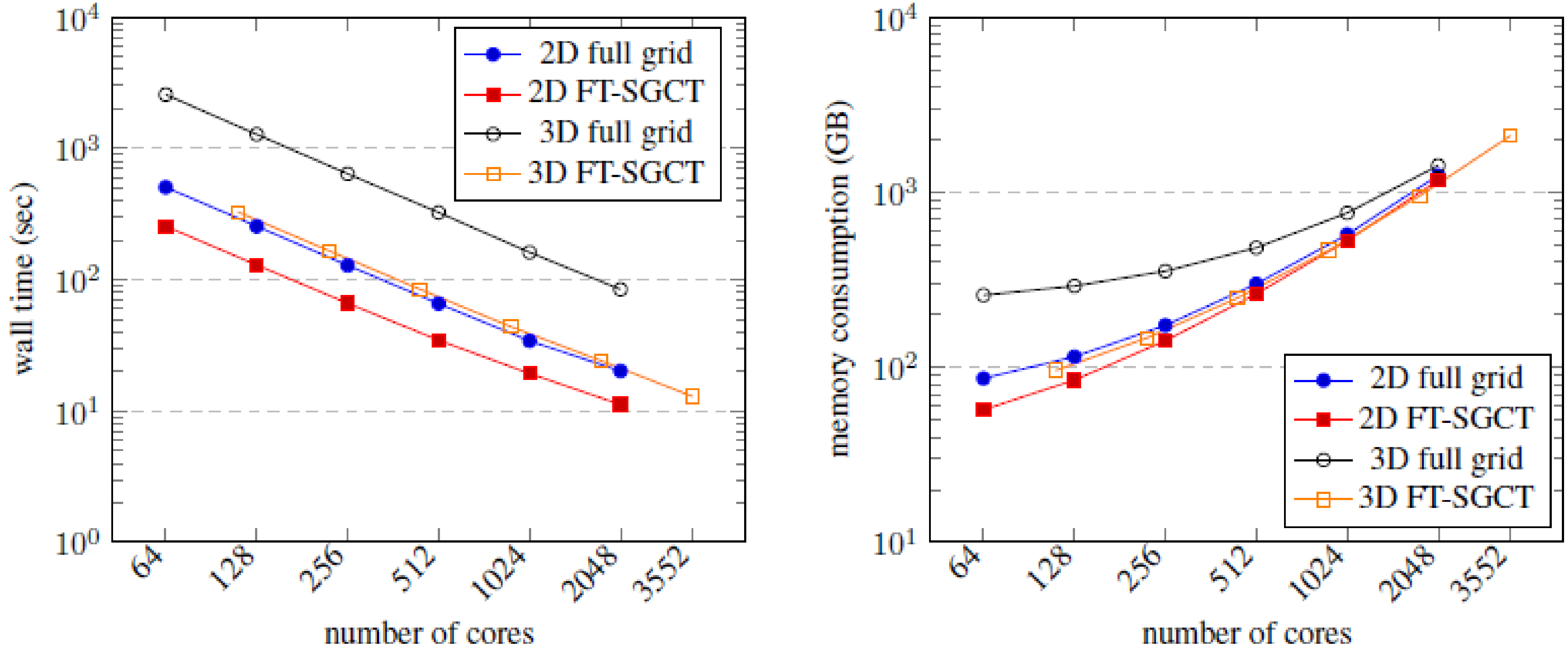
(b) expected relative recovery overhead for longer computation

- GENE has in-built checkpointing of `g_1` (note: very fast file system here!)
- WR/RD: read/write checkpoint, RM: relaunch MPI application
- RP/RN: recover process on same/different node
  - we should have $T_{RN} << T_{RM}$ (may improve in future ULFM MPI)

26 The Taxilla Lattice Boltzmann Method Application

- Taxila LBM is open source software for the LBM simulation of flow in porous and geometrically complex media
- highly scalable Fortran 90-based PetSc modular implementation
- chose a *bubble test*, in which one partially miscible fluid forms a bubble inside the other
- the density field is chosen for the output and used for the SGCT
- incorporating the SGCT similar to GENE, with $\{u_i\}$ corresponding to the `rho` array
    - default global communicators in `LBMCreate()` are replaced with C_i
    - process and data grid sizes are also passed in as parameters
    - local `rho` field extracted for SGCT after running `LBMRun()` using a shared pointer
    - periodic boundary conditions are used

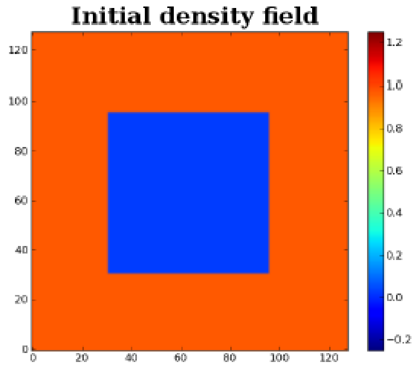
27 SGCT Taxilla LBM Performance and Accuracy



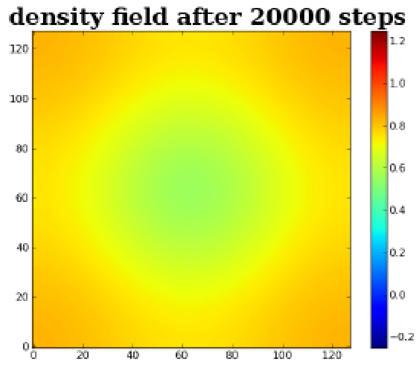
(a) overall execution time (b) overall memory usage

- 2D problem has $2^{13} \times 2^{13}$ full grid size with $l = 5$; 3D has $2^9 \times 2^9 \times 2^9$ and $l = 4$. 200 timesteps.
- accuracy (relative 1-norm difference to full grid) is $1.13E^{-2}$ and $3.98E^{-2}$, respectively

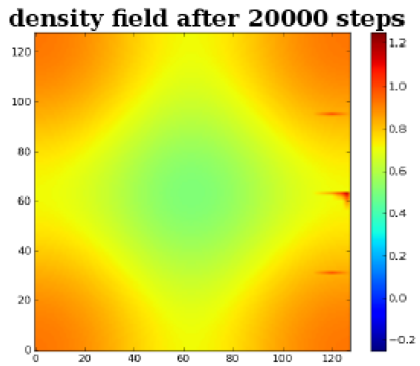
28 Taxilla Accuracy - Visualization



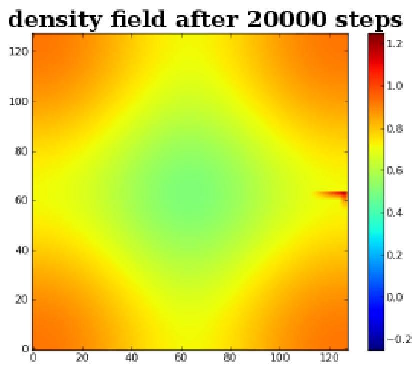
(a) initial full grid with no failure



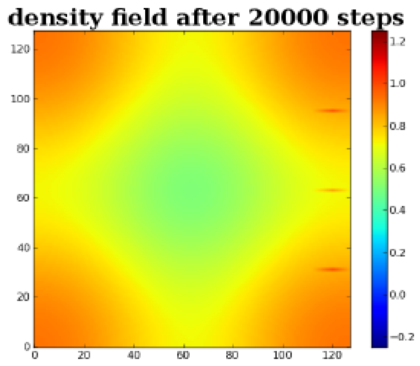
(b) full grid with no failure



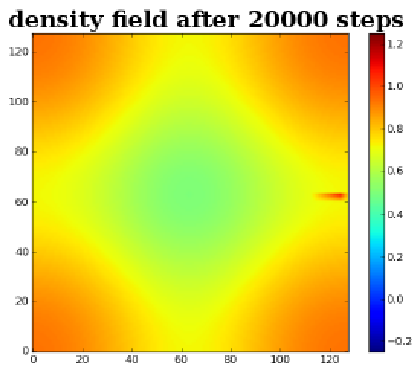
(c) combined grid with no failure (relative l_1 error is 5.0%)



(d) combined grid with processes on grid $G_{\underline{i}}$ with $\underline{i} = (1,3)$ fail (relative l_1 error is 5.07%)



(e) combined grid with processes on grid $G_{\underline{i}}$ with $\underline{i} = (3,1)$ and $(1,2)$ fail (relative l_1 error is 5.01%)



(f) combined grid with processes on grid $G_{\underline{i}}$ with $\underline{i} = (3,1), (1,3)$, and $(2,1)$ fail (relative l_1 error is 5.13%)

- comparison of density field for a $2^7 \times 2^7$ grid for an $l = 5$ SGCT
- smaller grid is used due to expense of computation

29 The Solid Fuel Ignition Application

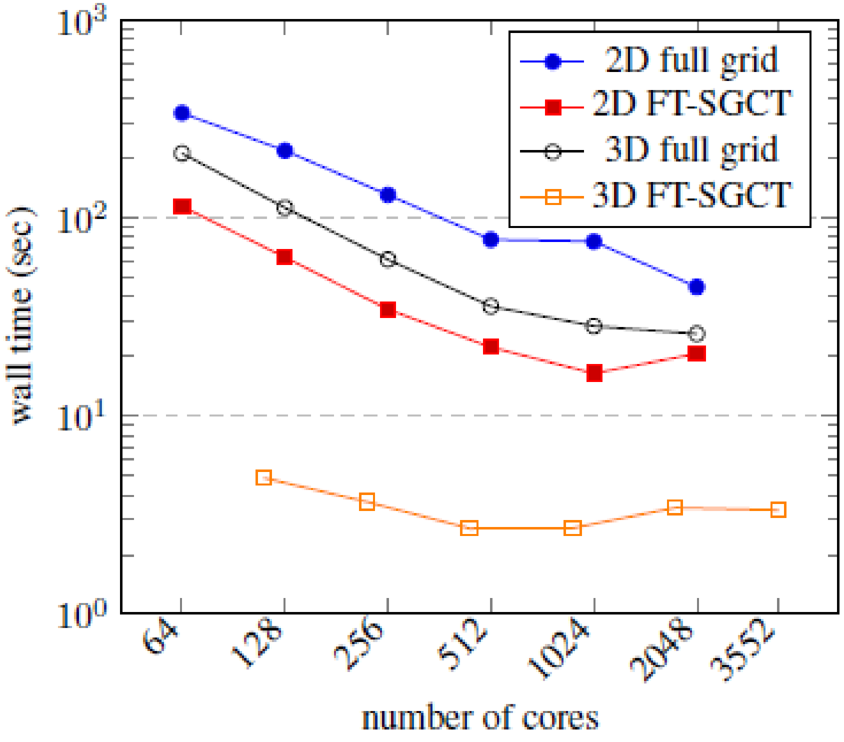
- involves solving the Bratu problem

$$-\Delta u(x,y,z) - \lambda \exp^{u(x,y,z)} = 0, 0 < x,y,z < 1$$

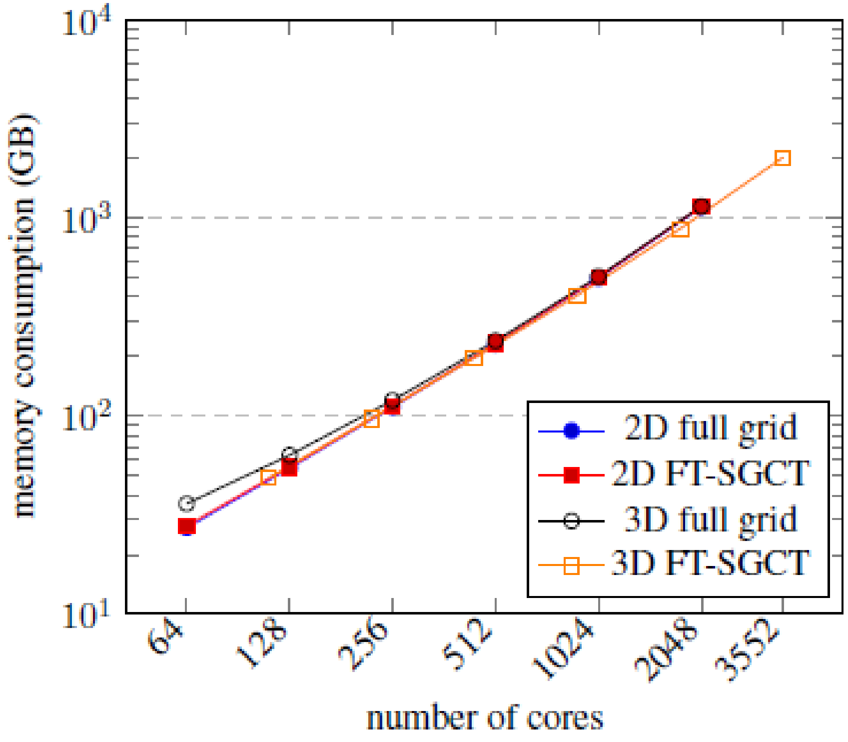
  where Δ is the Laplace operator and λ defines the degree of non-linearity

- a simpler application; also Fortran-90 PetSc code base
- incorporating the SGCT similar to Taxilla LBM, with $\{u_i\}$ corresponding to the `x` array in `SNESSolve()`
  - default global communicators in `SNESCreate()` and `DMDACreate2d()` are replaced with C_i
  - process and data grid sizes are also passed in as parameters to `DMDACreate2d()`
  - `c_get_sfi_field()` is called to pass the field to the SGCT codes
  - zero boundary conditions are used
- experiments used $\lambda = 6$ and Jacobian finite difference approximations

30 Solid Fuel Ignition: Performance and Accuracy



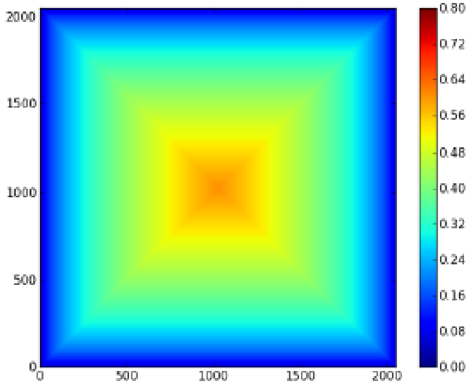
(a) overall execution time



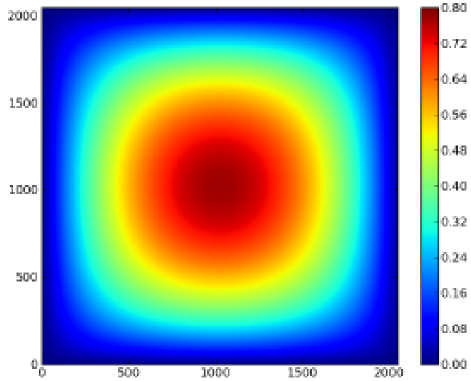
(b) overall memory usage

- 2D problem has $2^{11} \times 2^{11}$ full grid size with $l = 5$; 3D has $2^8 \times 2^8 \times 2^8$ and $l = 4$. 200 timesteps.
- 2D SGCT is $\approx 3\times$ faster, 3D $\approx 9\times$; accuracy is $1.27E^{-3}$ and $1.28E^{-3}$, respectively

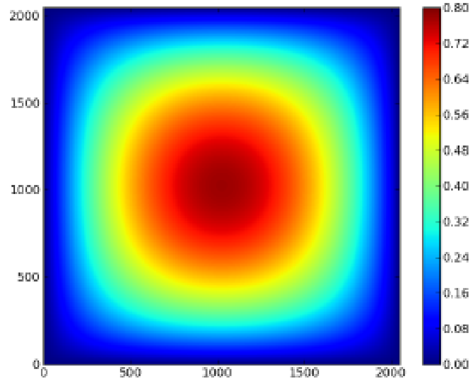
31 Solid Fuel Ignition: Accuracy - Visualization



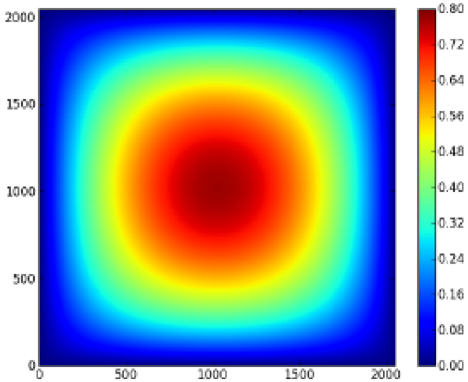
(a) initial full grid field with no failure



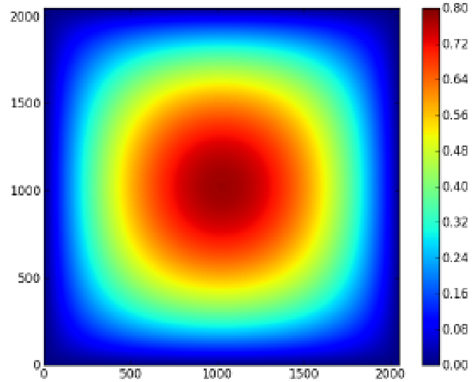
(b) full grid field with no failure



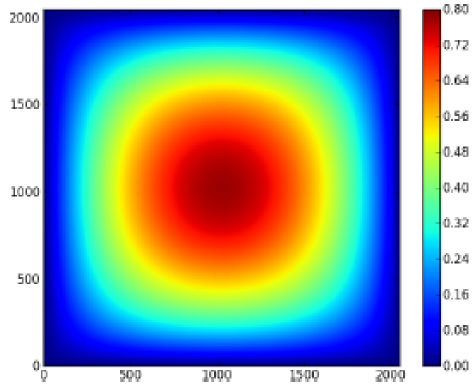
(c) combined grid field with no failure (relative l_1 error is 0.127%)



(d) combined grid field with processes on grid $G_{\underline{i}}$ with $\underline{i} = (1, 3)$ fail (relative l_1 error is 0.127%)



(e) combined grid field with processes on grid $G_{\underline{i}}$ with $\underline{i} = (3, 1)$ and $(1, 2)$ fail (relative l_1 error is 0.111%)



(f) combined grid field with processes on grid $G_{\underline{i}}$ with $\underline{i} = (2, 2), (0, 4)$, and $(2, 1)$ fail (relative l_1 error is 0.123%)

- comparison of field for a $2^{11} \times 2^{11}$ grid for an $l = 5$ SGCT

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32 Conclusions (I)

- the SGCT can give good accuracy-performance tradeoffs on a range of PDE simulations
  - with little extra computational cost, it can also be made fault-tolerant!
  - current ULFM MPI infrastructure is sufficient to support this
- the first fully parallel SGCT algorithms have been developed for 2&3D
  - complexity managed by vector arithmetic description
  - sparse grid data structured needed for direct algorithm, coalescing of supluses needed for the hierarchical
  - the direct algorithm is faster and is very scalable with core courts; also more scalable with level l and dimensionality d
    - if fields are already hierarchized, recommend de-hierarchizing and using the direct algorithm
  - algorithms designed for high resolution grids on smaller l and d
  - codes are available from http://users.cecs.anu.edu.au/~peter/projects/sgct

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33 Conclusions (II)

- a methodology to incorporate the SGCT has been proven on 3 complex pre-existing applications
  - relatively modest source code modifications required
  - a level of $l = 5$ ($l = 4$) for 2D (3D) gave $2\times$ (5–$9\times$) speed benefit for an ‘acceptable’ loss of accuracy
  - multiple SGCT can reduce error loss, especially for multiple failures
  - SGCT recovery time compares favorably to checkpointing
  - system is robust to multiple failures and combinations
  - Taxilla LBM and SFI are new (and successful) case studies!
- the SGCT is ready to support exascale computing!

34 Future Work

- some improvements can be made to the direct SGCT
  - removing restriction the SGCT process grid is a power of 2 can improve performance by a factor of ≤ 2
- test the methodology on other applications
  - solution must be ‘smooth’ for the SGCT to be effective
- can be extended to higher d; however, requires no more than 1 grid per process
- apply the SGCT to handle soft faults
  - detection may be challenging: ‘smearing’, application dependence
  - combine point-wise, in blocks or whole grids?
  - the hierarchical algorithm has a major advantage:
    common information in the component grids can be directly compared
  - more challenging time and memory requirements are likely

Thank You!! ...Questions??? Comments???

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Publications:

- Md Mohsin Ali, James Southern, Peter Strazdins and Brendan Harding, *Application Level Fault Recovery: Using Fault-Tolerant Open MPI in a PDE Solver*, Proceedings of the 2014 IEEE International Parallel & Distributed Processing Symposium Workshops, pp1169-1178, Pheonix, May 2014.
- Peter E. Strazdins, Md. Mohsin Ali, and Brendan Harding, *Highly Scalable Algorithms for the Sparse Grid Combination Technique*, Proceedings of the 2015 IEEE International Parallel & Distributed Processing Symposium Workshops, pp941–50, Hyderabad, May 2015.
- Md Mohsin Ali, Peter E. Strazdins, Brendan Harding, Markus Hegland, J. Walter Larson, *A Fault-Tolerant Gyrokinetic Plasma Application using the Sparse Grid Combination Technique*, Proceedings of the 2015 International Conference on High Performance Computing & Simulation (HPCS 2015), pp499-507, Amsterdam, July 2015. **(Outstanding Paper Award)**.
- 2 journal papers under preparation