Robust Solution of Partial Differential Equations Using Sparse Grid Combination Techniques

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

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1 Talk Overview

- overview of the associated project and the Open Petascale Library
- context: why we need new algorithms; methods of handling faults
- basic mathematical ideas: solution on multiple grids
- sparse grids and combination techniques
  - recovery methods for lost grids
  - experimental results on a 2-D advection solver
- prototype implementations in PDE solvers
  - modified map-reduce framework
  - integrated approach
- issues
  - fault detection, limitations
  - on applications of interest: ANUGA and GENE
- conclusions and future work

2 Overview of the ANU-FLE Petascale Algorithms Project

- investigate and develop new methods for solving first order hyperbolic PDEs of form $\frac{\partial u_i}{\partial t} = \nabla \cdot \mathbf{j_i}(\mathbf{u}) + s_i(\mathbf{u}), \quad i = 1, \ldots, d$
- co-developed with 2 applications in tsunami modelling & plasma physics
- aim to deliver scalability and resilience for very high levels of parallelism, with asynchronous computation, delivering:
  - scientific understanding of these new mathematical techniques
  - new techniques and software which demonstrates these techniques
- began mid 2011; as well as the co-investigators, team has 1 postdoc (Jay) and 3 PhD students (Brendan, Mohsin & Chris)
- broader collaboration with Fujitsu Labs Europe researchers
- part of Open Petascale Libraries Project (hosted by FLE)
  - advance numerical software for new generation of supercomputers
  - members include RIKEN, JAIST, NAG, Imperial College, UTK, UI, . . .

3 Why We Need Fault-tolerant Algorithms

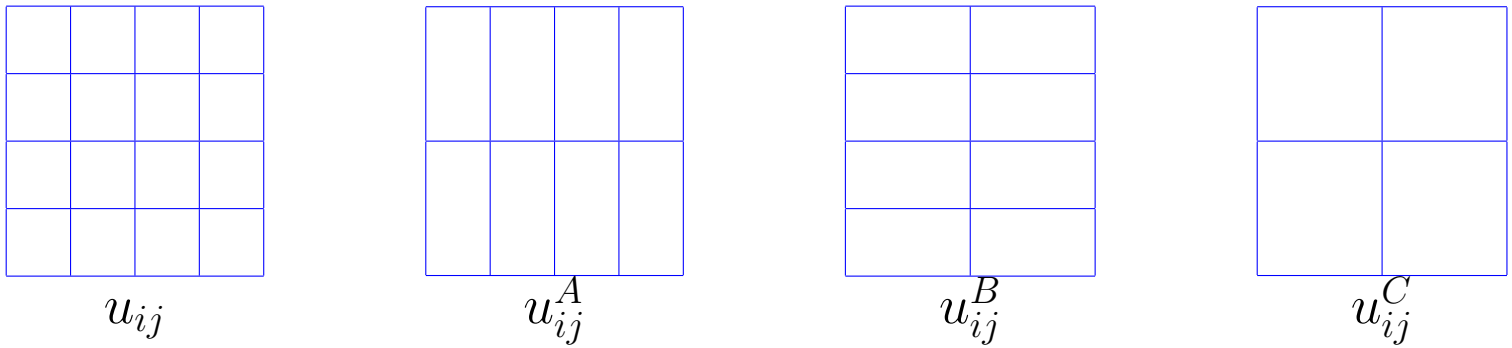
- Kei supercomputer developed by Fujitsu and RIKEN has 80,000 processors
  - connected by a sophisticated network (TOFU)
- as synchronization at this scale is expensive, we need fundamentally asynchronous algorithms
- need a new approach, relaxing computational dependencies and resilient against
  - missing data (not available at the right time)
  - errors (due to infrequent hard and soft faults)

4 Methods for Handling Faults

- checkpoint-restart (most common)
  - via I/O is not suitable for exascale (MTTI $\sim$ cost, I/O system prone to faults)
  - improved if not process-level – but requires application to implement
  - via memory is an improvement
- replication: typically 2 or 3 $\times$ redundancy
- failure avoidance (based on prediction from logged data)
  - not general
  - problem of false +ve and -ves
- algorithm-based fault tolerance (ABFT)
  - potential for lower redundancy, but can be hard to implement
  - can be 'oblivious' (preferable); otherwise requires detection & action

5 Robust Techniques for Time-dependent PDEs: Basic Ideas

- solve same problem on multiple different grids



u_{ij} u_{ij}^A u_{ij}^B u_{ij}^C

$$u_{11} \approx \gamma_A u_{11}^A + \gamma_B u_{11}^B + \gamma_C u_{11}^C$$ general formula

$$u_{11} \approx \tfrac{1}{2} u_{11}^A + \tfrac{1}{2} u_{11}^B - \tfrac{1}{4} u_{11}^C$$ high accuracy

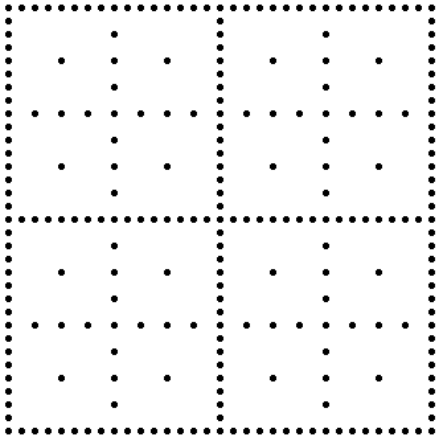
$$u_{11} \approx \tfrac{1}{2} u_{11}^B$$ if u_{11}^A not available

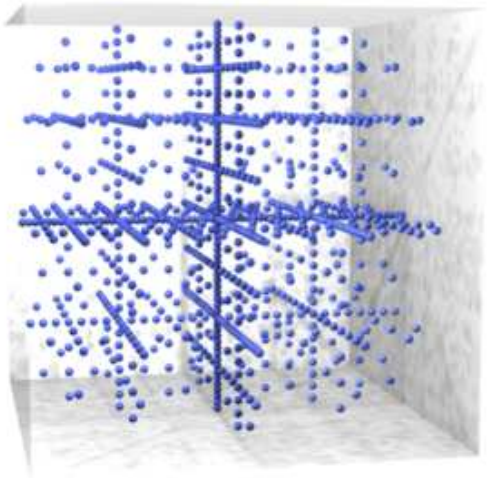
where $u_{11}^{[A,B,C]}$ is integral of u over top-left rectangle

- can use wavelet analysis and nonlinear approximation theory (derive error bounds)
- intend to develop new robust extrapolation techniques which are able to both correct errors and estimate missing data

6 Sparse Grids

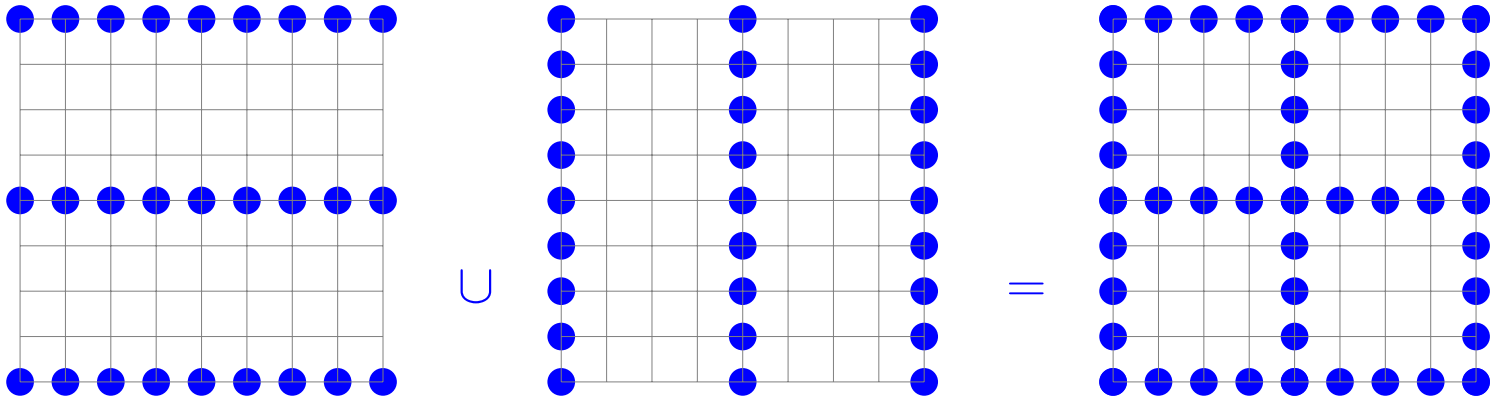
- introduced by Zenger (1991)
- for (regular) grids of dimension d having uniform resolution n in all dimensions, the number of grid points is n^d
  - known as the curse of dimensionality
- a sparse grid provides fine-scale resolution (n) in each dimension, but not at all places
  - the total number of grid points is $O(n \lg(n)^{d-1})$
  - 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



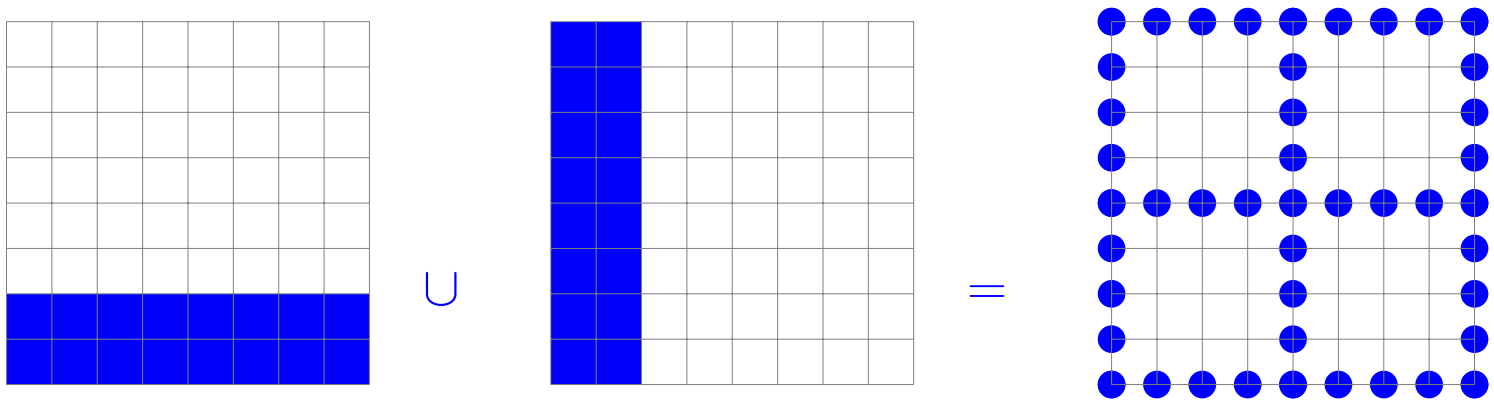


7 Sparse Grids: Geometric Construction

- a simple sparse grid from regular grids $(1,3)$ and $(3,1)$ (sizes $(2^1+1)\times(2^3+1)$ and $(2^3+1)\times(2^1+1)$)



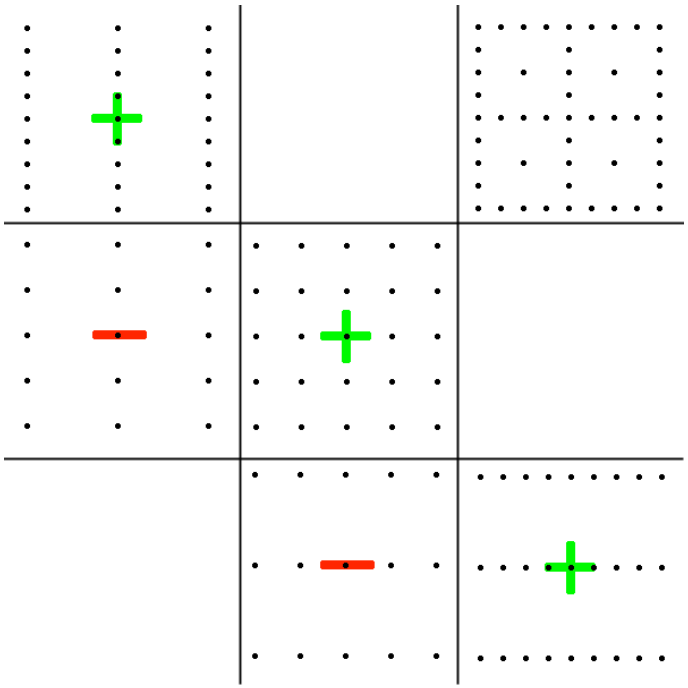
- sparse grid in frequency / scale space

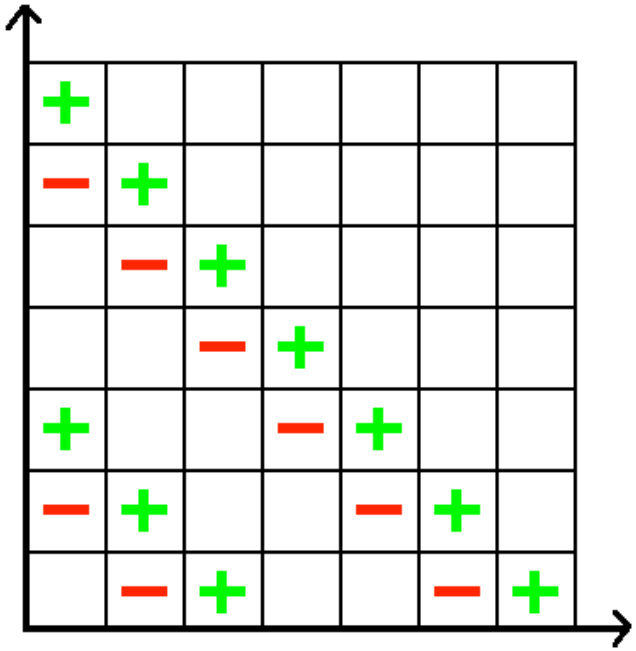


- captures fine scales in both dimensions but not joint fine scales

8 Combination Technique for Sparse Grids – 2D Case

- 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' $m = 4$, combine grids $(3,1)$, $(2,2)$ $(1,3)$ minus $(2,1)$, $(1,2)$



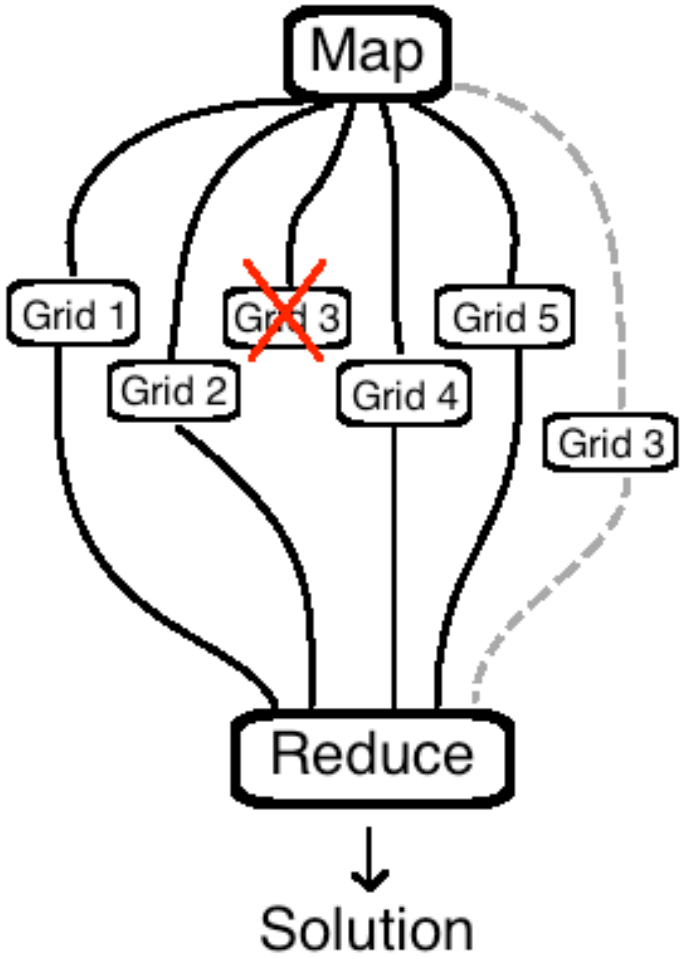


9 Combination Technique for Sparse Grids – General Case

- for 2D, combination technique of level m is
  $u_m^c(\mathbf{x}) = \Sigma_{i+j=m+1}\, u_{i,j}(\mathbf{x}) \;-\; \Sigma_{i+j=m}\, u_{i,j}(\mathbf{x})$
  - in practice, actual grid size for grid (i,j) can be $(2^{i+m_0}+1)\times(2^{j+n_0}+1)$, where $m_0, n_0 \geq 0$
- for d dimensions, classical combination technique of level $m \geq d-1$, is
  $u_m^c(\mathbf{x}) = \Sigma_{q=0}^{d-1}(-1)^q \binom{d-1}{q} \Sigma_{||\mathbf{i}||_1=m-q} u_{\mathbf{i}}(\mathbf{x})$ where $\mathbf{i} = (i_1, i_2, \ldots, i_d)$
- the number of sub-grids depends on d, m and the particular combination scheme
  - for classical combination, more than $d\binom{d-1}{q}$
  - typically, $O(10)$ for 2D, $O(10^4)$ for 6D
- solution via the combination technique can be expressed in terms of a map-reduce computation
  - map: solve for each $u_{\mathbf{i}}(\mathbf{x})$ for $m-d \leq ||\mathbf{i}||_1 \leq m$
  - reduce: add grids (with interpolation) with their respective coefficient

10 Robust Combination Techniques I: Recompute Lost Sub-grid

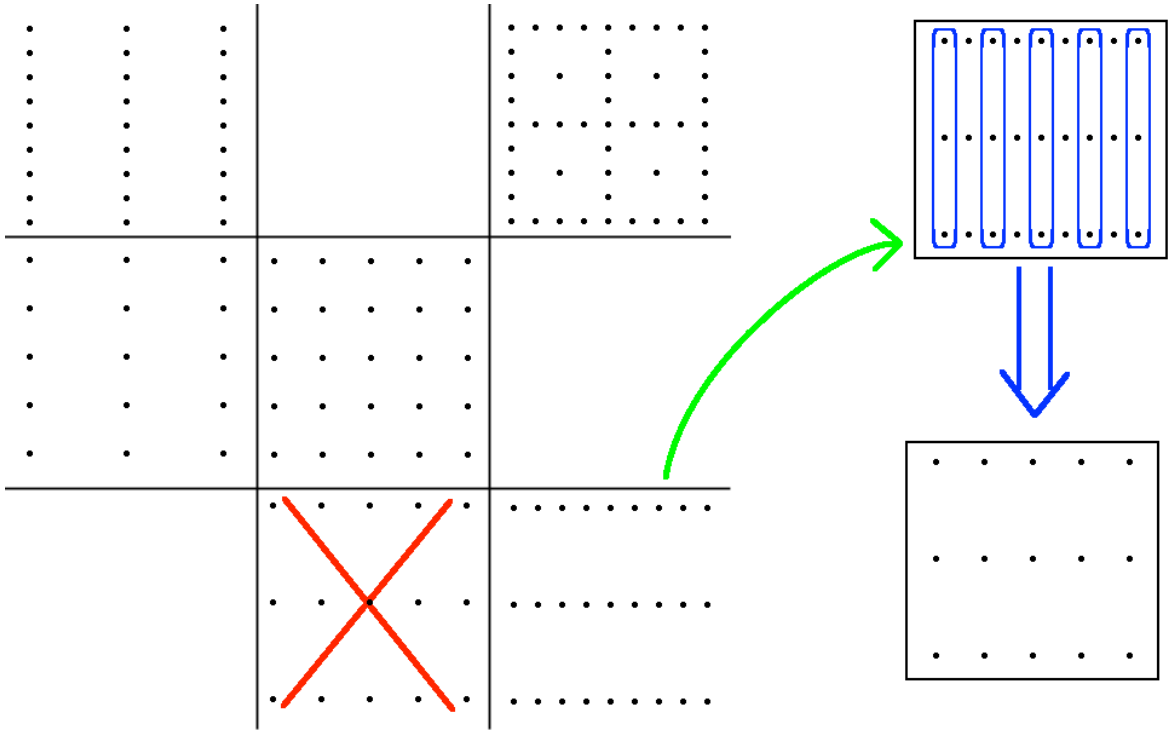
- in an FT map-reduce framework, can simply re-compute any failed map
- here, amounts to recomputing a sub-grid of $O(n)$ points,
  where $n \leq 2^m$
  - much less than re-computing the full $(O(n^d))$ or sparse $O(n \lg(n)^{d-1})$ grid solutions
- may be useful in a cloud / grid context
- this is a 'loss-less' method



11 Robust Combination Techniques II: Resample a Finer Sub-grid

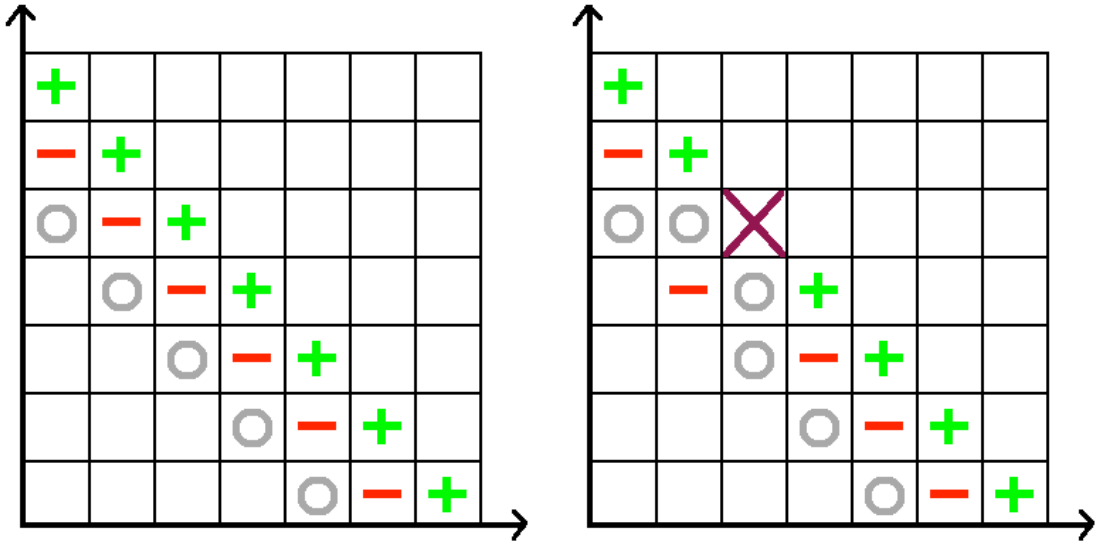
- on a finer sub-grid $\mathbf{i}$, i.e. $||\mathbf{i}||_1 < m$,
  there are at least d sub-grids which this is a subset

  - this grid can simply be recovered by re-sampling from any of these sub-grids $\mathbf{i}'$,
    where $i'_j \geq i_j$ for each $j = 1 \ldots d$
  - highly efficient
  - possibly a small loss of accuracy



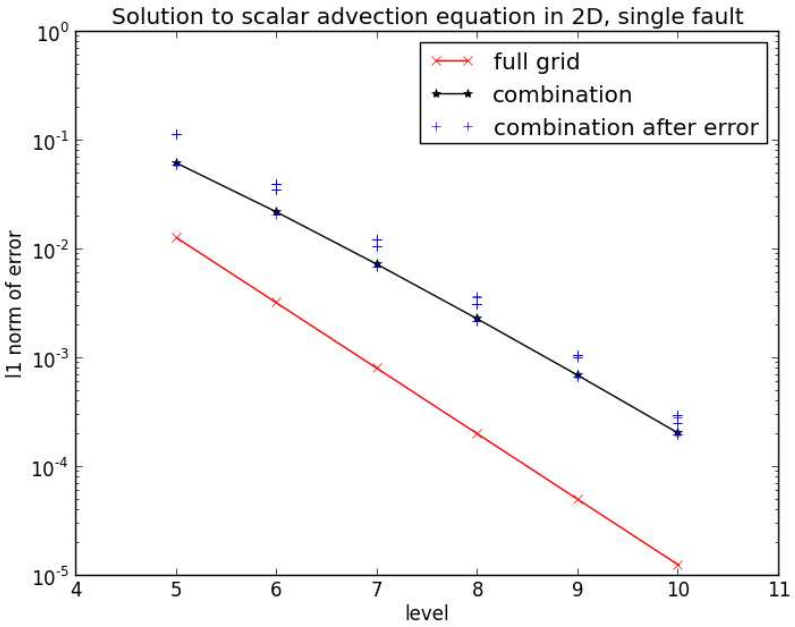
12 Robust Combination Techniques III: Extended Formula

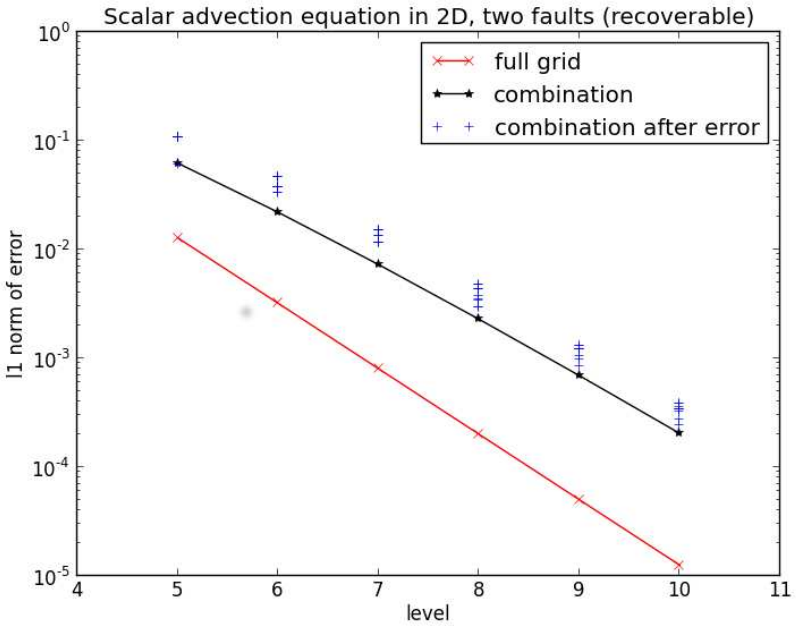
- uses extra set of smaller sub-grids with $||i||_1 = m - d$ (now $m \geq d$)
  - the redundancy from this is $< 1/(2(2^d - 1))$
- for a single failure on a sub-grid, can find a new combination formula with an inclusion/exclusion principle avoiding the failed sub-grid
- also works for many (but not all) cases of multiple failures
- if the failure is in one of the coarsest sub-grids, can recover this from the projection of the sparse grid combination



13 Experimental Results on 2-D Advection

- use $u_t + \mathbf{a} \cdot \nabla u = 0$, $a = (1, 1)$ on unit square, with $u_0(x, y) = \sin(2\pi x) \sin(2\pi y)$ (exact solution for $t = 0.5$ is u_0)



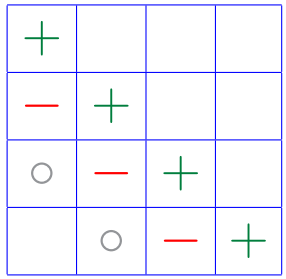


- error cases are within a factor of 3 of non-error sparse grid
- sparse grid solution with $4\times$ (max.) resolution has same errors as full grid, with less than $\frac{l+2}{2^{l-3}}$ of the work

14 Prototype Implementation I: Modified Map-Reduce

- recall sparse grid solution of PDEs fits in the map-reduce framework
  - map: compute solution on each sub-grid, producing <key, value> = <grid-index, (sub-grid-id, grid-value)> pairs
  - reduce (combination technique): at each point grid-index, add grid-value weighted by coefficient determined by sub-grid-id
- Hadoop could in principle provide a FT implementation, but not suitable
- instead, use an MPI-based framework based on $M \times N$ data transfers
  - create a pool of manager tasks which xc`MPI_spawn` processes of (possibly legacy) code solvers on each sub-grid
  - solvers must have an interface to transfer sub-grids to specified reduce processes
  - could use a 'heartbeat' mechanism to determine node failures, or more simply timeouts
  - determine the most appropriate combination formula and instruct reduce processes accordingly

15 Prototype Implementation II: Integrated Approach



- 48 process example:
  assign $+$, $-$, and $\circ$ sub-grids 8, 4 & 2 processes each
- repeatedly:
  - evolve system T_o time-step's, by repeatedly:
    - evolve sub-grids T_i time steps
    - check for failures (FT all-reduce); if any failures:
      - reconstruct (lost data from) failed sub-grid(s) from (partial) sparse grid via resampling or modified combination formula
      - re-spawn processes for failed sub-grids
  - gather sub-grids into a compete sparse grid & scatter back to sub-grids
    (can use a spatial decomposition over all processes)
- T_o determined from accuracy considerations; T_i by MTTI

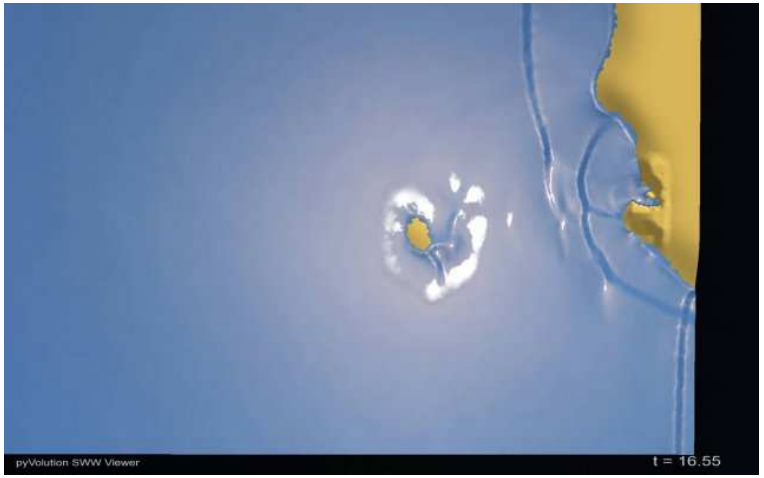
16 Issues in the Sparse Grid Approach

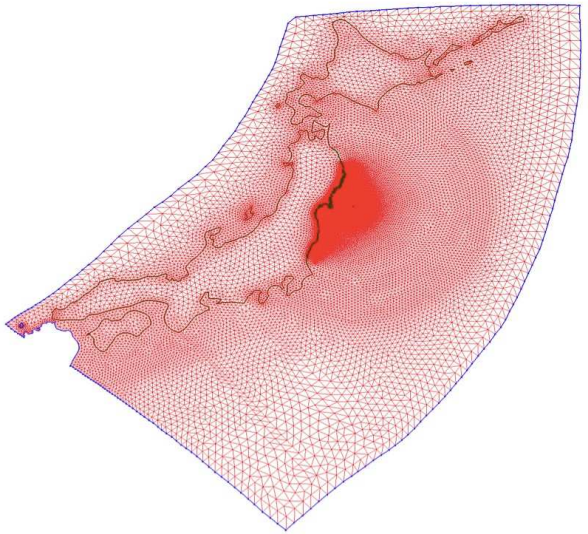
- while an ABFT technique, still fundamentally limited by MTTI
- full combination step is very communication-intensive! ($\Rightarrow$ largish T_o)
- handling of soft errors could be done at (see previous algorithm):
  - failure check step (locally check for outliers in each sub-grid)
  - when forming full sparse grid (full information available)

  Problem: delayed handling of soft errors $\Rightarrow$ smearing
- general limitations of the sparse grid technique
  - must be composed of regular grids
  - requires power of two grid (± 1) dimensions – wasteful, can be problematic
  - implementation of combination technique is very complex $\Rightarrow$ power of 2 number of processes per sub-grid

17 ANUGA Tsunami Propagation and Inundation Modelling

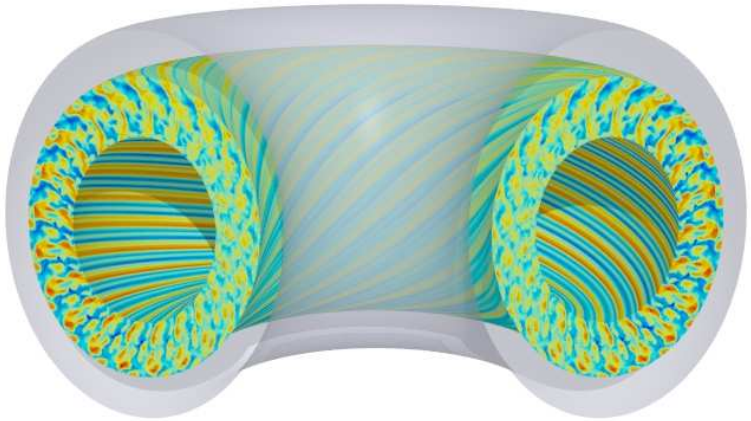
- website: ANUGA; open source: Python, C and MPI
- shallow water wave equation, takes into account friction & bed elevation
  - 2D triangles of variable size according to topography and interest
  - time step determined by triangle size and wave speed
- sim. on 40M cell Tohoku tsunami: super-lin. speedup to 512 cores on K
- open problem: define a theory for combining irregular meshes!!





18 Applications - GENE

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



- 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
  - physical phenomena well aligned to spatial co-ordinates

19 Conclusions and Future Work

- new mathematical methods have a great promise to the area
  - redundancy can improve accuracy and/or permit resilience
- sparse grid techniques can provide viable recovery methods for soft & hard faults
  - promising results for 2-D advection
- only some applications are suitable; GENE is but is very complex
  - advection is too ‘simple’ to scale; need something in-between
- complex infrastructure will be needed to support a FT implementation!
- current status:
  - two approaches for implementation in the design stage
  - developing an efficient non-FT combination algorithm
  - simulation of faults, under a realistic fault model; analyzing how likely modified combination formula can be applied
- future work includes exploring higher dimensional (3D +) problems

Thank You!!

. . . Questions???