Concurrent Divide-and-Conquer Library
with Petascale Electromagnetics Applications

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Background

- Particle In Cell (PIC) in a sentence: solve Faraday and Ampere laws for electromagnetic fields and get current closure from set of particles accelerated by Lorentz force
- For the purpose of this talk: think FDTD EM + explicit current-source calculation
- Two main uses for implicit field updates
  - Allow time steps beyond CFL limit, $\Delta_t > \Delta_x / c$
  - Numerical dissipation can suppress particle and other numerical noise (grid heating)

- VORPAL PIC code used by INCITE project (PI'd by Geddes) and OFES SciDAC project (PI'd by Bonoli), etc.
- Explicit (Yee) field update has excellent scalability
- Original implicit field update was added to VORPAL in February 2004

Bowers vs. ZCZ ADI implicit field update

- Two implicit field updates were on shortlist
  - Bowers adds damping terms to Faraday and Ampere laws
    - $\nabla \times \mathbf{F} \rightarrow \nabla \times [(1 + \tau_F\, \partial_t)\mathbf{F}]$, for $\mathbf{F} = \mathbf{E}, \mathbf{B}$
    - Use Crank-Nicholson (CN) time discretization
    - Damping times $\tau_{E,B}$ correspond to implicitness parameters
    - $\tau_E = \tau_B = \Delta_t/2 \Rightarrow$ fully implicit
    - $\tau_E = \tau_B = -\Delta_t/2 \Rightarrow$ fully explicit
    - Numerical dispersion well analyzed by Bowers
  - ZCZ ADI (Alternating Direction Implicit)
    - *"Toward the Development of a Three-Dimensional Unconditionally Stable Finite-Difference Time-Domain Method"*, F. Zheng, Z. Chen and J. Zhang, IEEE Trans. on Microwave Theory and Techniques **48** (2000) 1550
    - Not charge conserving!
- Bowers came out ahead

Implementation of Bowers implicit field update in VORPAL

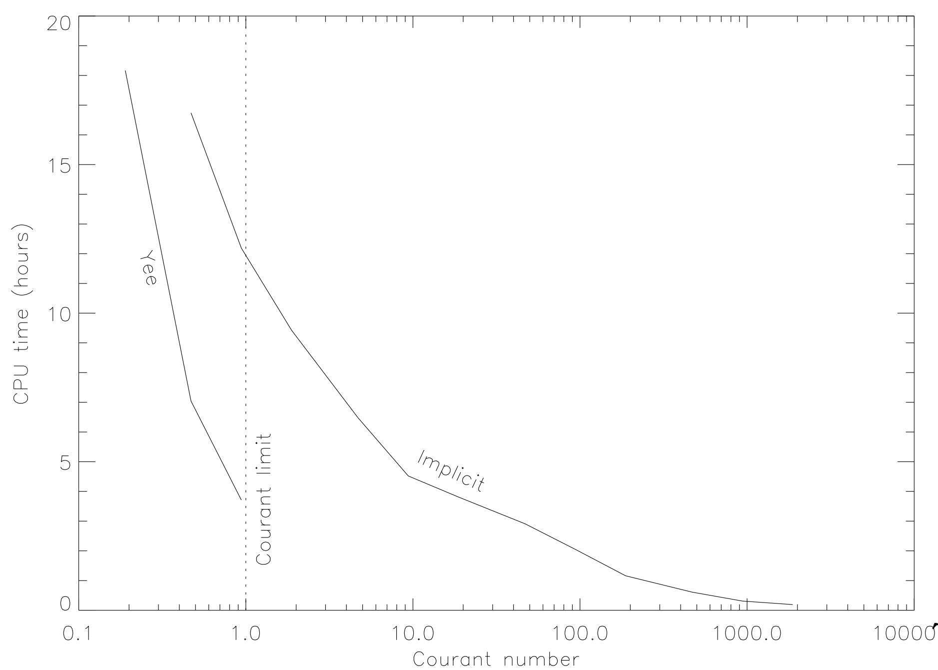
- An electrostatic (ES) field update had just been added to VORPAL
  - Trilinos/Aztec used for linear solve
- Bowers implicit field update implemented making maximal reuse of existing ES solver
- Implementation was done in a couple of weeks as evidenced by SVN log of main class file:

```
Thu 05 Feb 12:59:02 Adding new class for the implicit field
solver.
Thu 05 Feb 13:41:20 First iteration of changes.
Fri 06 Feb 19:35:00 Flipped the indices around.
Mon 09 Feb 19:42:19 Coded up the coefficient matrix.
Tue 10 Feb 11:46:06 Bug fix in the coefficient matrix.
continued...
```

Implementation of Bowers implicit field update in VORPAL

```
Tue 10 Feb 12:25:05 Added the proper expressions for the
coefficient-matrix elements (including Bowers' damping
coefficient, etc.).
Tue 10 Feb 19:56:03 This afternoon's changes.
Wed 11 Feb 15:46:34 Coded up the right-hand side.
Wed 11 Feb 18:53:23 The core code should now be pretty much
complete (setting up coefficient matrix and RHS, updating the
field).
Thu 12 Feb 19:13:53 The code now builds.
Mon 16 Feb 18:26:35 Bugfix.  Now it builds with HAVE_AZTEC
defined.
Fri 20 Feb 11:18:07 Misc bugfixes.
Tue 24 Feb 21:49:24 Minor changes, still having convergence
problems with the iterative solver.
Wed 25 Feb 19:44:23 Several critical bugfixes!  Implicit solver
now seems to work.
```


Performance of Bowers implicit field update in VORPAL



Performance of Bowers implicit field update in VORPAL

- $\sim 3\times$ slower than explicit at CFL limit
- $2-3\times$ more memory used by field (can't update in place)
- Good numerical stability (convergence for CFL number above 10^3)
- However, $\sim$ 10 iterations in 1D, $\sim$ 40 in 2D, $\sim$ 400 in 3D!
- Became orphaned when OFES SBIR Phase I project didn't go to Phase II
- Has only been clearly superior in particle-dominated (hundreds per cell) 2D simulations
- Numerical dispersion not suitable for suppressing grid heating
- Concern about scalability due to global solve
- Multigrid preconditioning recently tried, but found ineffective

Recent developments on Maxwell solvers using Alternating Direction Implicit (ADI)

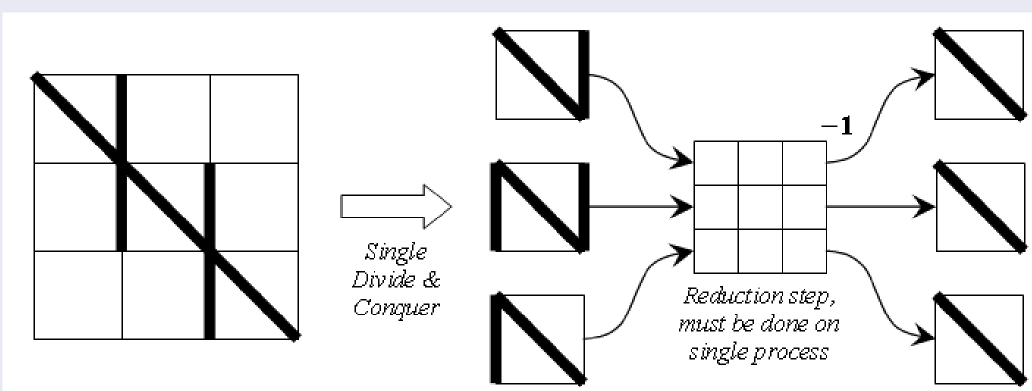
- Seminal paper by ZCZ mentioned above with first unconditionally stable ADI field update
- Work at Tech-X over last year by Smithe, Cary and Carlsson
  - Improved version of ZCZ that is Space-Charge Conserving (SCC) ADI
  - SCC ADI with "perfect dispersion" (avoids numerical Cherenkov radiation)
- Should lead to high-fidelity solutions
- But does it scale?!?

ADI seems to have largely fallen out of favor

- Was supposedly popular for elliptic problems before multigrid became dominant
- Divide timestep into substeps and Alternate which single Direction is Implicit in each substep
- Reduces single global solve into series of small tridiagonal solves
- Could make implicit field update more like explicit update (Yee) in terms of communication needs (keep field data local) and scalability
- Bondelli introduced parallel algorithm for solving tridiagonal system: Divide & Conquer

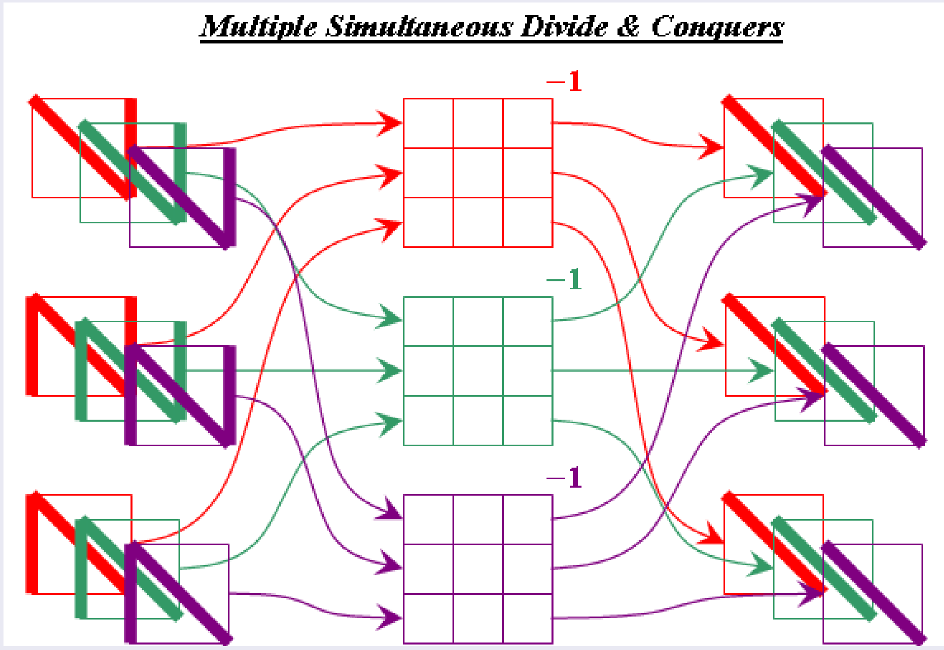
ADI non-trivial to parallelize efficiently

- Use Divide & Conquer to parallelize solve of tridiagonal system
  - Begin solve in parallel
  - Sequential bottleneck
  - Finish solve in parallel



Concurrent Divide-and-Conquer

- Keep multiple tridiagonal solves in flight simultaneously to overlap communication with computation



Scalability formula can be derived

- Let C_{1D} be number of cells in one direction, so that $C_{3D} = C_{1D}^3$
- Let N_{1D} be number of processors in one direction, so that $N_{3D} = N_{1D}^3$
- Let τ_{cell} = time it takes to do backsolve of a single cell
- Let $\tau_{latency}$ = time it takes to receive a message
- Then the maximum number of cell-rows that can be done simultaneously by a processor is $N_{cellrows} = C_{1D}^2/N_{1D}^2$
- A processors share of the common-matrix-inversions is therefore, $N_{immediate} = N_{cellrows}/N_{1D}$
- The number of cells in a single-processor's backsolve is $N_{cellsSolved} = C_{1D}/N_{1D}$

So immediately following a processor's common-matrix-inversion-and-send on the $N_{immediate}$ matrices, it can proceed with $N_{immediate}$ backsolves, which will take a time:

$$N_{immediate} N_{cellsSolved} \tau_{cell}$$

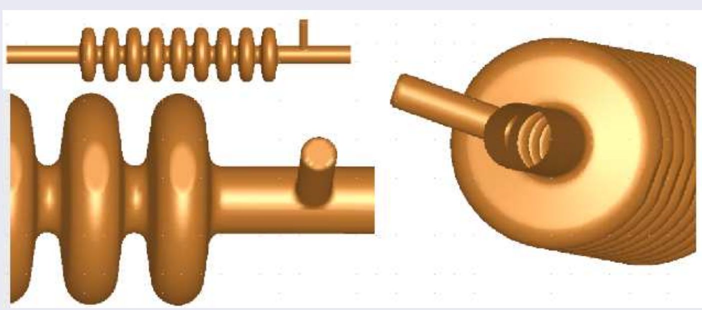
to perform. This must exceed $\tau_{latency}$ in order to ensure that there is no idle processor time.

Might be possible to achieve good scaling on biggest available machines

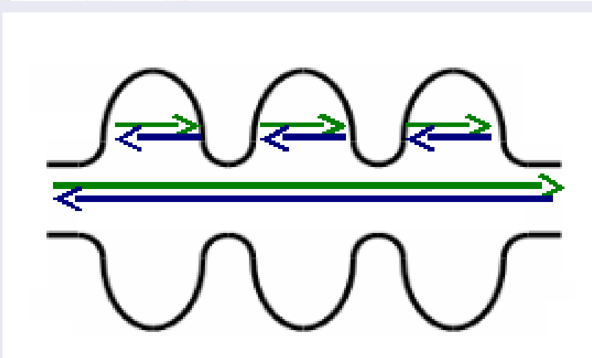
$$N_{immediate} N_{cellsSolved} \tau_{cell} \geq \tau_{latency}$$
$$(N_{cellrows}/N_{1D})(C_{1D}/N_{1D})\tau_{cell} \geq \tau_{latency}$$
$$((C_{1D}^2/N_{1D}^2)/N_{1D})(C_{1D}/N_{1D})\tau_{cell} \geq \tau_{latency}$$
$$(C_{1D}^3/N_{1D}^4)\tau_{cell} \geq \tau_{latency}$$
$$(C_{3D}/N_{3D}^{4/3})\tau_{cell} \geq \tau_{latency}$$
$$N_{3D} \leq (C_{3D}\tau_{cell}/\tau_{latency})^{3/4}$$

With $\tau_{latency} = 100\tau_{cell}$ and a billion cells ($10^3 \times 10^3 \times 10^3$), it would then be possible to scale beyond 10^5 processors.

ADI can simplify handling of complex boundaries



ILC SRF cavity



ADI in ILC SRF cavity

How do we get an efficient and portable implementation?

We have recieved an ASCR SBIR Phase I grant to implement a prototype ADI library and prove the scalability of our new SCC ADI algorithm

- Must balance efficient implementation vs. portability
- MPI1 or MPI2? Or UPC?
  - MPI2 becoming ubiquitous
  - Any new killer features?
- Multilevel parallelism with MPI/OpenMP?
  - gcc4.2 supports OpenMP
  - BlueGene/P nodes are SMP
- More library dependencies can be added to VORPAL only if there are very compelling reasons
- Other considerations for efficient implementation?