Numerical Relativity and Numerical Analysis

Global Problems in Mathematical Relativity
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What do Numerical Relativists Want from Mathematical Relativists?

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RESPECT!!!

Goals of Numerical Relativity

- Astrophysics
  - Waveforms for LIGO
- Physics
  - Understanding of strong field gravity
- Mathematics
  - Understanding of solution space of Einstein equations and its relationship to other sets of PDEs in mathematical physics

Numerical Relativity as Computational Science

- Field driven to large extent by HARDWARE and SOFTWARE developments
- Hardware developments
  - 1995 Supercomputer (UT Austin), 8-processor CRAY Y-MP vector machine, peak speed about 2 Gflop/s; could get on order of 1000 hours of CPU PER YEAR, effective sustained rate of about 0.02 Gflop/s
  - 2005 Supercomputer (UBC/WestGrid), 1680-processor IBM, peak speed about 4000 Gflop/s; individual researcher may be running on > 100 processors continuously; sustained rate of over 200 Gflop/s
- Increase in raw computing speed of some 4 orders of magnitude in 10 years

Numerical Relativity as IDEAL Subfield of Computational Science

- How do we evaluate potential for numerical computation in a given field, as well as compare with other fields?
- Try to assess "scientific return on computational investment"
- Rate of return will depend on many things: among most important are
  - Potential for genuinely NEW discoveries (vs confirming one's intuition, or supplying Nth decimal digit of effect computed in simpler context)
  - SCALING PROPERTIES of computation (what is incremental cost of improving accuracy of calculation; can numerical analysis genuinely SOLVE problem in practical fashion)

Potential for New Discoveries in Numerical Relativity

- Very high, due to
  - Nature of field equations/solutions: nonlinear, time-dependent, geometrically complicated
  - Lack of experimental/observational results and attendant "physical intuition": i.e. simulation is to assume role of experiments

Scaling Properties in Numerical Relativity

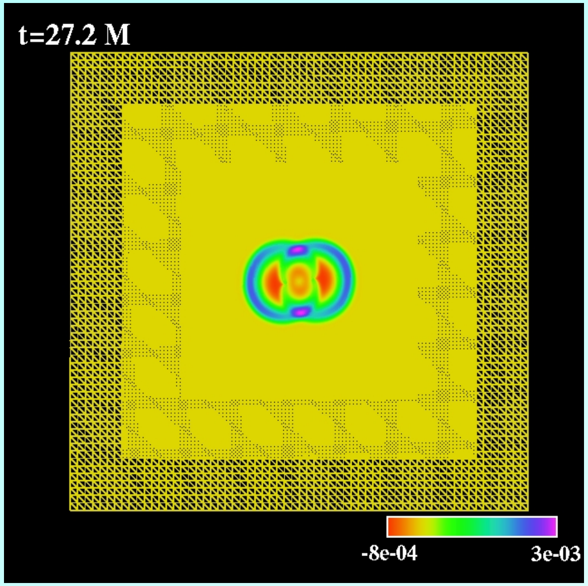
- Also near ideal, in principle, due to
  - CLASSICAL, DETERMINISTIC nature of field equations and solutions
    - Examination of properties of even a SINGLE solution (of a binary merger, e.g.) makes sense
    - Generally no need for "ensembles" (weather forecasting, e.g.), not hampered by slow convergence due to statistical effects (similar issues arise in many problems of QUANTUM origin)
  - Expected SMOOTHNESS of gravitational fields (modulo physical singularities), even though "dynamical range" (ratio of largest to smallest length/time scales in solution), may be very large

Scaling Properties in Numerical Relativity

- Exploiting smoothness (Achi Brandt late 1970's on)
  - By fully exploiting smoothness in solutions, can, in principle, design and implement algorithms for which the decrease in solution error is essentially exponential in the amount of computational work invested (spectral accuracy)
  - In general, thinking in terms of, e.g., finite difference methods, such algorithms will need to be
    - Multi-level: employ a variety of discretization scales, h
    - Adaptive: optimal h will be a LOCAL quantity, determined by features of solution, and "on the fly" (i.e. adaptively)
  - MLAT: Multi-level Adaptive Techniques

Sample Adaptive Mesh Refinement Structure from One of Pretorius' Recent Binary BH calculations

1



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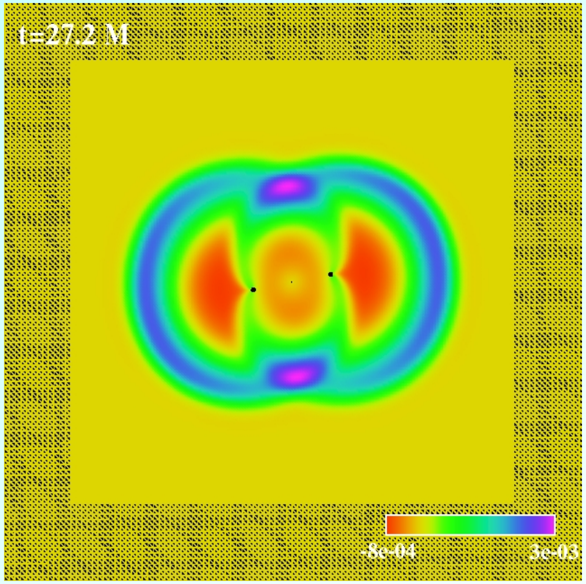

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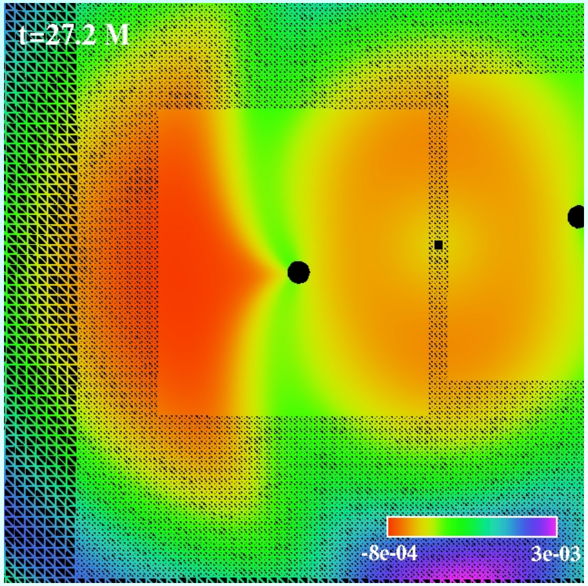

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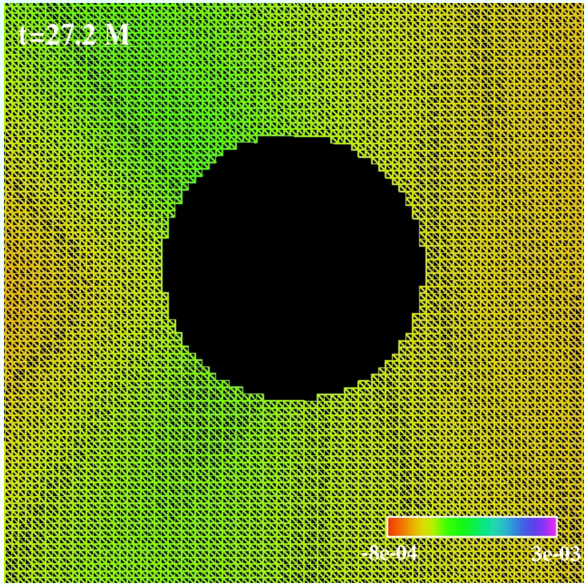

Scaling Properties and Optimizations

- "Traditional" optimizations (examples)
  - Reducing number of steps needed in given iterative process
  - Looking for "best possible" difference scheme of given order

- Essentially irrelevant in NR relative to use of technique with "right" scaling
  - Computational cost must scale linearly as function of "physical process" in system, i.e. must be O(N) where N is the number of (discrete) degrees of freedom, and where we have a scheme in place (MLAT) such that each new DOF yields approximately the same "resolution" to the scheme

Don't sweat the "constant factors"!!

- If you have an O(N) method, and I have a FASTER O(N) method, then chances are very good that we will be able to do basically the same science, irrespective of how much faster my method is than yours for a given calculation
  - "Curse of dimensionality": in 3+1 calculations N scales as the 4^{th} power of (inverse) resolution
  - No "magic resolution" (discretization scale) at which problem becomes "solved"; "slop" of 2-3 in h becomes 10-100 in cost of simulation; likely to swamp traditional optimizations (e.g. PREDICTABLY slow progress in unigrid computations over past decade or so)
  - Convergence tests MANDATORY; again range in cost of calculations in changing resolution from, e.g., h -> h/2 -> h/4 likely to mask gains from usual type of optimization

Solutions vs Equations

- In linear problems, equations and solutions are more or less equivalent, and (modulo boundary conditions), likely to be able to deduce much about solution space from structure of equations
  - "Finite" complexity in solution space
- NOT the case in non-linear problems
  - Solution phenomenology potentially arbitrarily complex, and little if any hope of understanding/predicting phenomenology from structure of equations per se
- View already implicit in discussion of MLAT techniques

Role of Model Problems

- Has been tendency in both numerical and mathematical camps to assume that we can lay out a sequence of increasingly complicated/realistic model problems to get us from where we are to where we want to go

- Argument is that we have to start somewhere, might as well start from simple cases, and, in addition, if we CAN'T solve simple cases, clearly CAN'T solve more complicated ones

Role of Model Problems

- Can identify two basic types of model problems
  - Ones in which "model" aspect is a result of imposing symmetries, or discarding some physical elements thought to be relatively inessential to problematic physical/mathematical behaviour (GOOD)
  - Ones in which "model" aspect is a result of adopting distinct but related physical/mathematical setup, such as use of scalar/vector/… fields instead of Einstein field (NOT SO GOOD, AT LEAST ON BASIS OF TRACK RECORD)
    - MANY instances where techniques/approach for "toy" problems involving scalar/Maxwell fields, e.g., work very well, but then do not extend readily to gravitational case
    - Again, relates to focus on EQUATIONS rather than on SOLUTIONS

Role of Formalism Development

- Even in early 1990's I was complaining that the proposed number of formalisms/approaches for calculations in numerical relativity seemed large given the number of practicing numerical relativists
- Since then situation has only "worsened" in that respect, but, HAVE been significant and very welcome developments from the "mathematical side"
  - Understanding of well-posedness (hyperbolicity, etc.) for both the (pure) Cauchy as, well as mixed initial-boundary value problems

Role of Formalism Development

- Again, new formulations of Einstein's equations tends to focus ON the equations, rather than on the solutions
  - From computational point of view, ONLY thing in which we are interested in the first instance is the solution, and its computational cost
  - Both the solution and the cost are fixed by the PHYSICS of the particular scenario under consideration, NOT by the structure of the equations, and in general, cannot expect there to be "magic bullet" approaches (including, e.g. coordinate choices), for broad classes of solutions
  - More promising approach: General, flexible, adaptive algorithms to "rough out" solution space, followed by solution-tailored techniques, ansatz etc. for higher accuracy

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Why don't you do more numerical analysis?

Numerical Analysis and Numerical Relativity

- Researchers tend to use terms ANALYTIC and NUMERICAL as antonyms, as is "we would like to solve this equation analytically, but we can't, so we resort to numerical methods"

- I object vehemently to this usage on the grounds that
  1. Fundamentally, analysis is that branch of mathematics concerned with approximation
  2. Numerical analysis IS just that; i.e. analysis carried out using (only) arithmetic operations, but in such as fashion that, in principle, statements concerning the continuum can be made

Numerical Analysis as Applied Mathematics

- Nature of implementation (i.e. computer programming), and in particular the relatively small percentage of a typical NR "code" devoted to the numerical analysis per se, tends to obscure the fact that, an algorithm is A MATHEMATICAL CONSTRUCT, with specific mathematical properties that themselves can be analyzed

- Failure to view "code" as applied mathematics can lead to "code twiddling" in which researchers start to view the program per se as the fundamental object, with potentially disastrous consequences for the mathematical properties of the algorithm per se

- Culturally, at least, mathematical relativity community has much to impart to (neophyte) numerical relativists, in terms of rigour of approach which is no less important "at finite resolution" than it is in the continuum

Getting Into The Numerical Game: The Good News

- The numerical analysis used, at least to date, in NR is not very "deep"
  - Field is still "underdeveloped" in terms of methodology relative to similar areas of computational science, including, e.g. computational fluid dyamics
  - Many, if not most, major advances in NR (in terms of genuinely NEW solutions) have been made on the basis of "ad hoc" efforts, rather than those built up systematically from previous efforts

Example of "ad hoc" approach
Pretorius' Generalized Harmonic Code

- Key features of approach that buck tradition
  - Uses continuum version of the equations based on generalized harmonic coordinates rather than 3+1 approach
  - Uses spatially compactified domain, plus numerical dissipation to "quench" outgoing radiation at large distances
  - Differences equations directly in second-order form (does not recast into system that is first order in time)

Getting Into the Numerical Game: The Bad News

- At some point, do have to "code", and irrespective of the fundamentally mathematical nature of numerical analysis "code", this task is not always commensurate with the mathematician's taste and/or experience
- The most interesting/pressing (astrophysically-motivated) problems, such as binary inspiral and merger ARE messy and complicated, and take a LONG time (person-years, minimum) to set up and push through
- Requires access to appropriate computer resources

Symbiosis between Mathematical and Numerical Camps

- Perhaps the most appealing and logical form of interaction to which we can aspire
- Analogy with traditional view of experimentalist/theorist interaction with physicist
  - Numericist (experimentalist) deduces new behaviour phenomenologically (i.e. via numerical experiments)
  - Mathematician (theorist) extracts key insight from experiments than allow him/her to make conjectures concerning more general situations, adopt specific ansatz that leads to "analytic" (i.e. "closed form") solution, etc.

Symbiosis

- Have already seen this type of development in context of
  - Bartnik-McKinnon Einstein-Yang-Mills solutions
  - Critical collapse
- Have also seen examples of traditional mathematical developments being exploited by numericists
  - Garfinkle's recent numerical work on BKL conjecture in fully 3+1 D cosmologies based on "continuum" work due to Uggla et al

Potential for Contributions from Mathematical Relativity vis a vis the Numerical Relativity "Laundry List of Concerns"

- New continuum formulations [INDETERMINATE!]
- Constraint violations and related stability issues [HIGH, e.g. Pretorius' incorporation of constraint damping following Gundlach et al]
- Coordinate conditions [LOW, without tight coupling to one or more "codes"]
- Excision and related techniques [LOW]
- Analysis and interpretation of solutions [HIGH]
- Outer boundary conditions and other issues related to mixed initial-boundary value problems [LOW, predict that compactification will become method of choice]
- Stability of finite difference equations, given continuum stability [HIGH; see work by LSU group]
- "Extremely strong field initial data" [HIGH; issues related to existence and uniqueness of elliptic systems]

Conclusions

- A realizable ideal would involve efforts by both camps to move to more common ground
  - "Numericists" need to focus on more "mathematical approach" so that it is clear to those not doing the calculations precisely what is and what isn't working
  - "Mathematicians" need to focus more on moving at least part of their research programs into the numerical domain, including an attempt to engage in "real" problems, as well as model problems, that, interesting as they may be mathematically, may not bear directly on the solution of the more realistic scenarios