OF BLACK HOLES AND BEOWULFS

- Numerical Relativity: Goals and Challenges
- Equations of Motion
  - Time-independent
  - Time-dependent and Berger & Oliger AMR
- Critical Phenomena in Gravitational Collapse
- Infrastructure for Parallel Computations
- The `vn.physics.ubc.ca` Beowulf Cluster

Matthew W. Choptuik, UBC, CIAR & UT Austin

Department of Applied Mathematics Seminar
University of Washington, Seattle WA, December 7, 1999

Supported by NSERC, CIAR, CFI and NSF PHY9722068

Standard prefix: laplace.physics.ubc.ca:/People/matt/

Current Group

- At UBC
  - Matt Choptuik
  - Jason Ventrella UT Austin PhD student
  - Frans Pretorius PhD student
  - Inaki Olabarrieta MSc student
  - Kevin Lai Phd student
  - Roman Petryk Phd student as of 01/00
- At UT Austin
  - Scott Hawley PhD student
  - Ethan Honda PhD student
  - Scott Noble PhD student

Collaborators

- Bill Unruh
- Steve Liebling LIU faculty
- Eric Hirschmann LIU faculty
- Dave Neilsen UT Austin postdoc
- Luis Lehner UT Austin postdoc
- Mijan Huq Penn State research associate
- Dale Choi Drexel postdoc
- Carsten Gundlach Southampton, UK faculty
- Pablo Laguna Penn State faculty
- David Garfinkle Oakland U faculty
- Richard Matzner UT faculty
- Scott Klasky PPL research scientist

Numerical Relativity
Goals

Simulation of space-time without and with sources
Simulation of the gravitational field without and with sources

- Astrophysically relevant, dynamical, gravitational-radiation-producing spacetimes of particular interest,
  Must solve field equations in 3 space-dimensions plus time

- Physical Requirements for Efficient Radiation
  - (Large) masses confined to regions comparable in size to their Schwarzschild radii, R_S:

$$R_S = \frac{2G}{c^2} M$$

$$\frac{2G}{c^2} = 1.5 \times 10^{-27} \, \frac{\mathsf{m}}{\mathsf{kg}} = 3.0 \, \frac{\mathsf{km}}{M_\odot}$$

$$G = 6.67 \times 10^{-11} \mathsf{N\ m}^2/\mathsf{kg}^2 \qquad c = 3.00 \times 10^8 \mathsf{m/s}$$

R_S for Earth is about 1 cm!

  - Internal redistribution of significant fraction of energy at speeds approaching speed of light, c

LIGO Site 1: Hanford WA

(http://www.ligo-wa.caltech.edu/)

LIGO ≡ Laser Interferometer Gravitational-Wave Observatory

- Some Vital Statistics
  - Interferometer arms: 4 km
  - Sensitivity band: ≈ 30 to 1000 Hz
  - Phase I sensitivity: $\delta L/L \approx 1.0 \times 10^{-21}$
  - Phase II sensitivity: $\delta L/L \approx 1.0 \times 10^{-23}$

LIGO Site 2: Livingston LA

(http://www.ligo-la.caltech.edu/)

Numerical Relativity
Goals

- Ideal Candidates—"Compact Binaries"
  - Black hole–black hole binary (for BH, $R = R_S$)
  - Black hole–neutron star binary
  - Neutron star–neutron star binary

- Not-so-astrophysically relevant but physically motivated model problems also of interest, focus of my past research
  - No experimental GR
  - Possibility for "computational laboratories"
  - Good vehicle for infrastructure & algorithm development

Typical Model Problem

- Reduced spatial dimensionality (spherical, $1 + 1$, axisymmetric, $2 + 1$)
- "Simple" matter: typically scalar field instead of perfect fluid
- Key non-linear features retained (e.g. black hole formation)

Numerical Relativity
Challenges

- Large computational requirements
  - Back-of-the-envelope estimate for single 2 BH collision: 1 CPU week on 1 Tflop/s system
- Physical interpretation of results (incl. visualization)
  - Large number of dynamical variables
  - Dynamical vbls tend to be tensor components, so so often have no intrinsic physical interpretation *per se*
  - No "lab" for intuition
- Coordinate Freedom
  - Prescription for coordinatization of space-time must be given, can not assume to be known *a prioir*, as in non-general-relativistic dynamics.
  - Bad prescription of coordinates can (and often does!) lead to encounters with physical or coordinate singularities.
- Singularity Avoidance
  - BH space-times generically contain physical singularities; must be avoided or dealt with in a special fashion
- STABILITY (Convergence)

Equations of Motion (Schematic, No Matter)

- Fundamental variables: all functions of $(x, y, z, t))$
  Latin indices $i,\ j,\ \cdots$ range over $1, 2, 3$

$g_{ij},\ \ K_{ij}$ (6 + 6 = 12 fields) $\alpha,\ \ \beta^i$ (1 + 3 = 4 fields)

- Evolution equations: ("hyperbolic", use 4 to 12)

$$\frac{\partial g_{ij}}{\partial t} = -2\alpha K_{ij} + D_i\,\beta_j + D_j\,\beta_i$$

$$\frac{\partial K_{ij}}{\partial t} = \mathcal{L}_\beta K_{ij} - D_i D_j \alpha + \alpha \left(R_{ij} - 2K_{ik}K^k{}_j + K_{ij}K \right)$$

  where R_{ij} is the 3-Ricci tensor, $K \equiv K^i{}_i$, $\mathcal{L}_\beta$ is the Lie (convective) derivative along β^i, and D_i is a covariant derivative

- Constraint equations: ("elliptic", use 0 to 4)

$$\mathcal{C}_\mu[g_{ij}, K_{ij}] = 0 \qquad \mu = 0, 1, 2, 3$$

- Coordinate conditions: (algebraic,elliptic,hyperbolic, need 4)

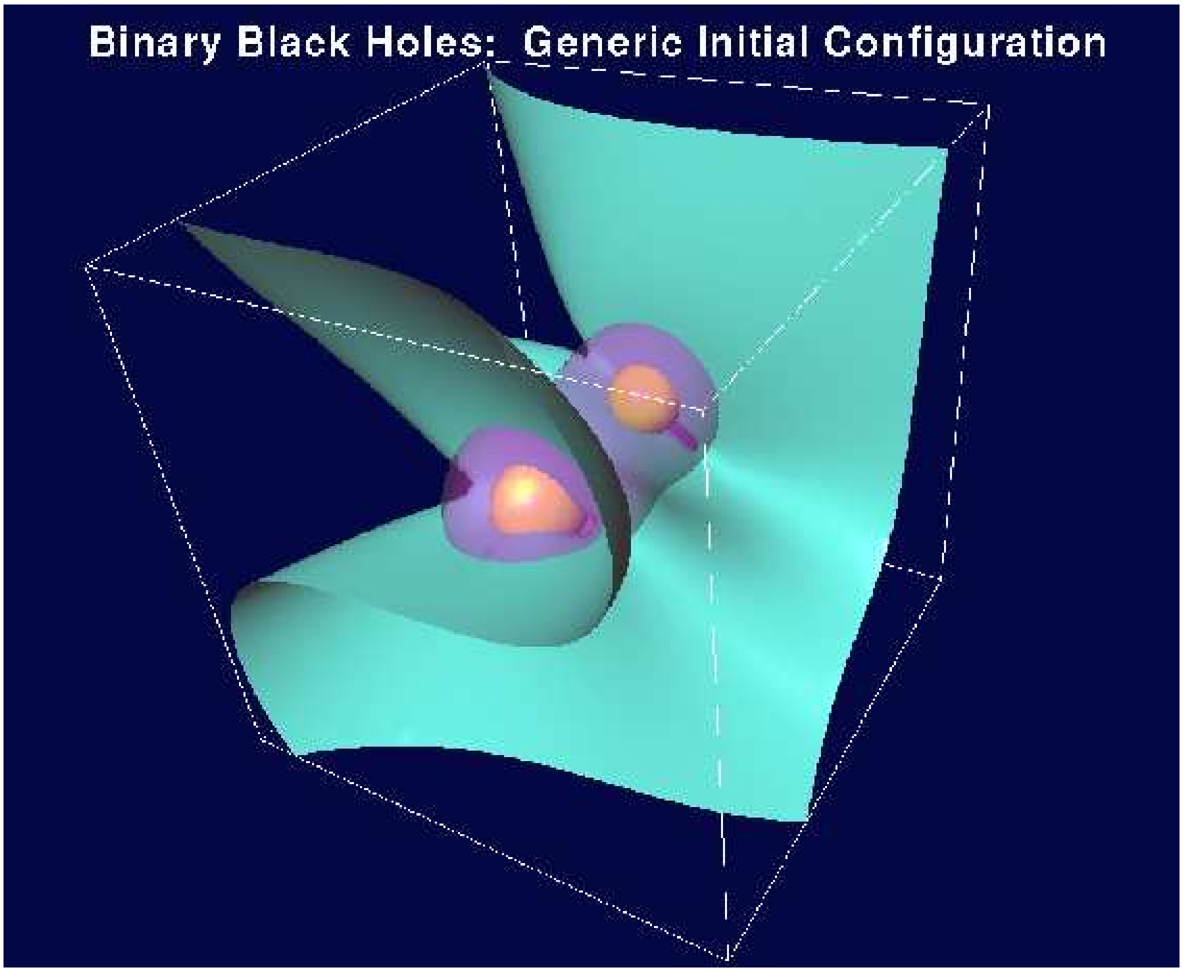
$$\mathcal{F}_\mu[\alpha, \beta^i; g_{ij}, K_{ij}] = 0$$

Equations of Motion
(Time-independent)

- Constraint equations must be satisfied by initial data (i.e. at $t = 0$
  - Industry developed over past 15 yrs for solving IVP for 2-BH problems
  - State-of-the-art quite advanced, typically uses multigrid in “body-adapted” coordinates, ICGC and relatives also widely used
  - Parts per million accuracy possible via Richardson extrapolation techniques
- Constraint equations can be used at $t \neq 0$ in lieu of evolution equations for certain dynamical variables (constrained evolution)
- Coordinate conditions often result in time-independent equations for kinematical variables α, β^i
- Observation: Even when “best available” algorithms are used, solution of “elliptics” often dominates state-of-the-art NR simulations

Visualization of Initial Data for 2 Black Holes

(Cook *et al*, *Phys. Rev. D*, 1993)



Equations of Motion
(Time-dependent)

$$\frac{\partial g_{ij}}{\partial t} = -2\alpha K_{ij} + D_i\,\beta_j + D_j\,\beta_i$$

$$\frac{\partial K_{ij}}{\partial t} = \mathcal{L}_\beta K_{ij} - D_i D_j \alpha + \alpha\left(R_{ij} - 2K_{ik}K^k{}_j + K_{ij}K\right)$$

- Many basic mathematical questions concerning structure of these specific equations (3 + 1 equations) remain, in particular, in general they are not rigorously hyperbolic

- Much recent work aimed at finding genuinely hyperbolic formulations; some promising results, but no current clear advantage relative to suitably massaged 3 + 1 equations

- Community tends to use $O(h^2)$ finite-differencing techniques on global (uniform) mesh
  - "Crank-Nicholson" schemes currently popular for 3 + 1 equations, typically solved iteratively
  - Standard methods for flux-laws can be used with hyperbolic formulations (Lax-Wendroff, McCormack, $\cdots$)

- (IN)STABILITY remains chief problem, particularly in conjunction with inner (black holes) and outer boundaries

Equations of Motion

Berger & Oliger Style AMR

Berger & Oliger *JCP* **53** (1984) 484–512

- Typical black hole problem requires significant dynamical range

$$\lambda_{\mathrm{radiation}} \sim 100\ R_{\mathrm{BH}}$$

- Some form of adaptive mesh refinement will be crucial for efficient 3-D computations

- Strategy: Implement *some* sufficient algorithm, don't worry if it isn't optimally efficient as long as scaling of computational time with "physical process" is roughly linear.

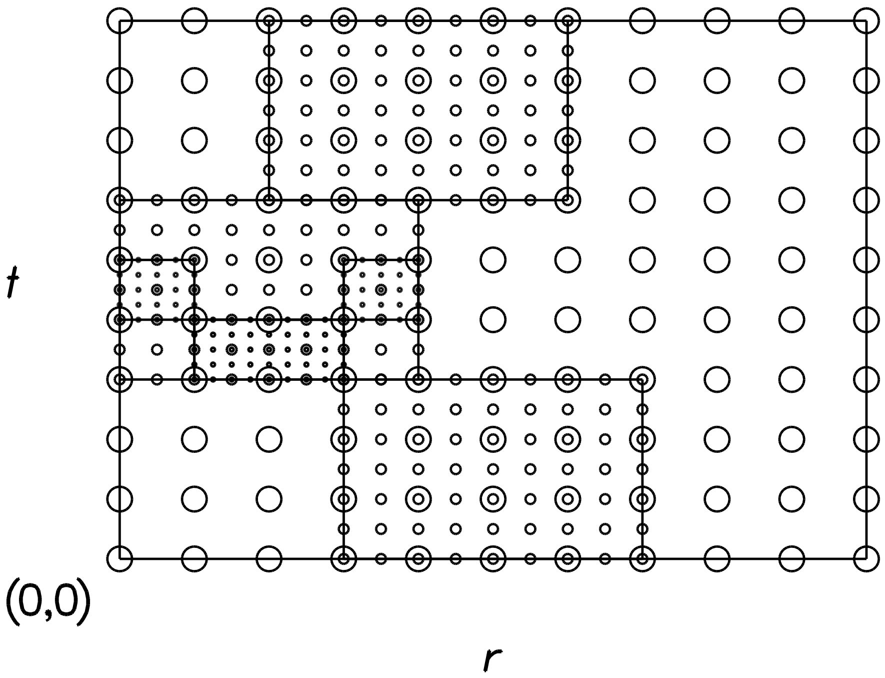
- "Minimal" Berger & Oliger algorithm (no rotation of sub-grids) arguably sufficient provided features of interest (needing resolution) remain predominantly volume-filling

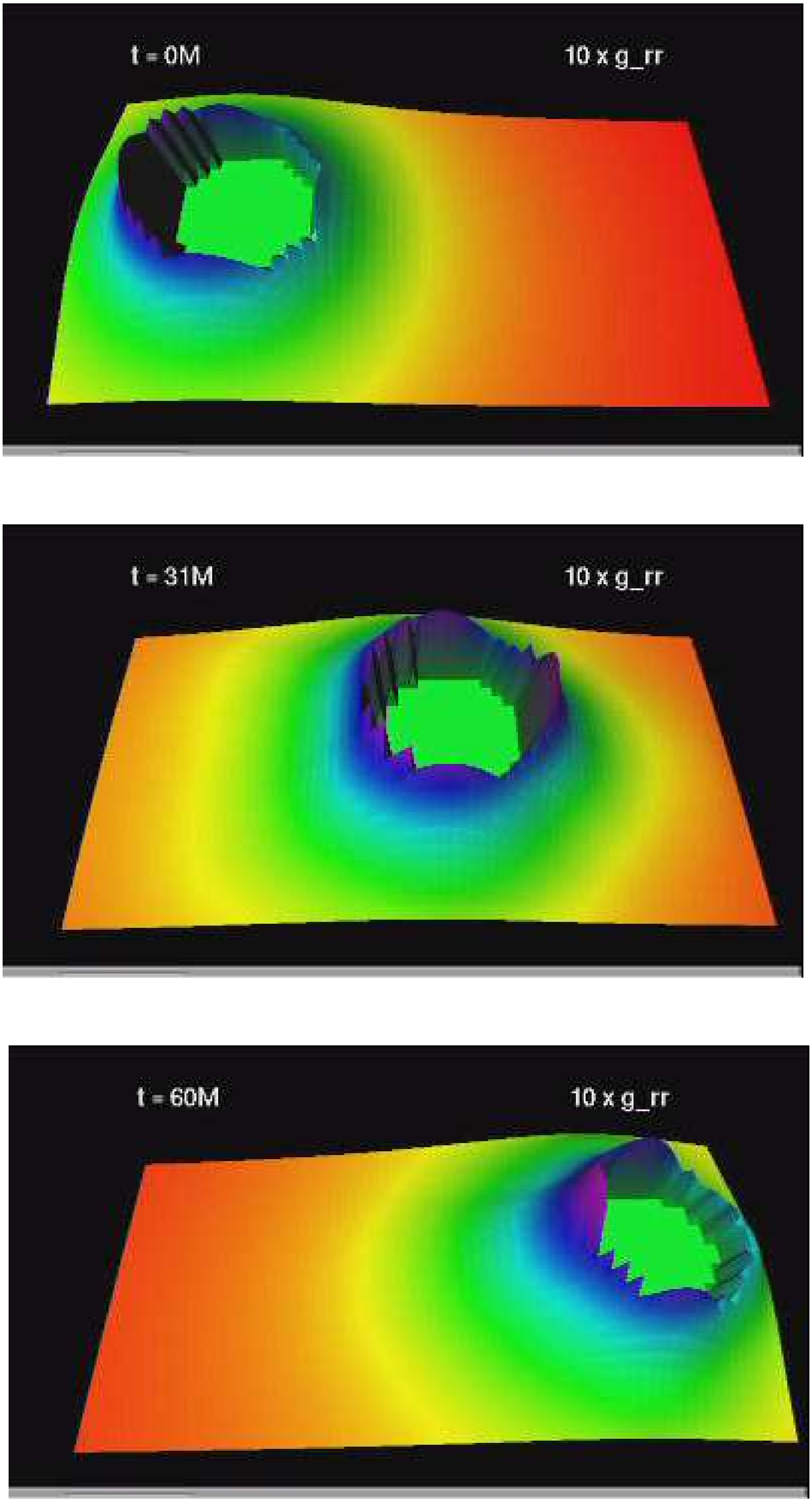
- Expected to be the case for general black hole interactions

- Considerable past and current activity in numerical relativity aimed at implementing and exploiting Berger & Oliger AMR

Schematic Adaptive–Mesh Structure

2 : 1 Refinement in Space and Time

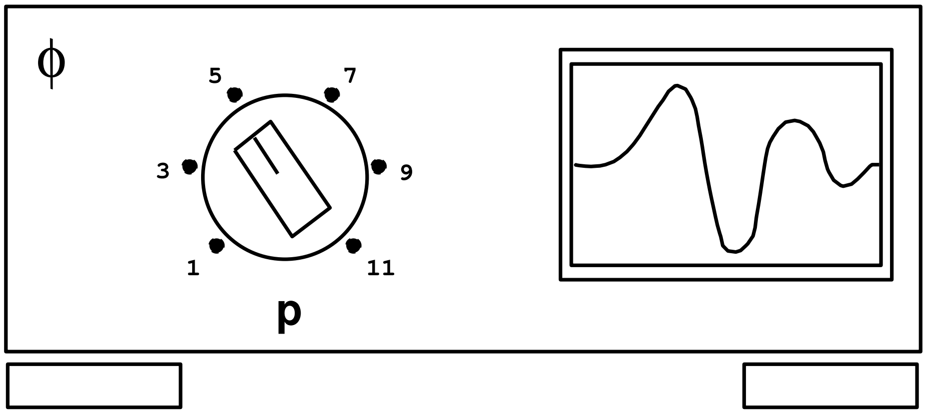




t = 0M
10 x g_rr
t = 31M
10 x g_rr
t = 60M
10 x g_rr

Critical Phenomena in Gravitational Collapse
The Game

- Consider parametrized families of collapse solutions
- Parameter, p, controls degree of self-gravitation in evolution



- Demand that family "interpolates" between flat spacetimes and spacetimes containing black holes:
  - Low setting: no black hole forms
  - High setting: black hole forms

Black hole formation "turns on" at some threshold value $p^\star$

Phenomena in near-threshold regime $\equiv$ *Critical Phenomena*

Critical Phenomena in Gravitational Collapse
Model Problem: Weak Field Behaviour (Linear Waves)

- Spherical symmetry: coordinates (t, r, θ, φ), no dependence on θ or φ

- Metric: ("geometric units": $G = c = 1$)

$$ds^2 = -dt^2 + dr^2 + r^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right)$$

- Scalar field equation of motion:

$$\Box\phi = 0 \quad \Longrightarrow \quad \frac{\partial^2}{\partial t^2}(r\phi) = \frac{\partial^2}{\partial r^2}(r\phi)$$

- General solution: ingoing & outgoing waves:

$$r\phi(r,t) \sim u(r+t) + v(r-t)$$

- Initial data: give ingoing profile, $f(r)$, outgoing profile, $g(r)$

$$\begin{aligned} r\phi(r,0) &= f(r) + g(r) \\ \frac{\partial}{\partial t} r\phi(r,0) &= f'(r) - g'(r) \end{aligned}$$

Critical Phenomena in Gravitational Collapse
Model Problem: Strong Field Behaviour

- Metric: In a particular coordinate system (generalization of Schwarzschild system)

$$ds^2 = -\alpha^2(r,t)\; dt^2 + a^2(r,t)\; dr^2 + r^2\left(d\theta^2 + \sin^2\theta\, d\varphi^2\right)$$

- (Auxiliary) scalar field variables:

$$\Phi(r,t) \equiv \frac{\partial \phi}{\partial r}(r,t) \qquad\qquad \Pi(r,t) \equiv \frac{a}{\alpha}\frac{\partial \phi}{\partial t}(r,t)$$

Critical Phenomena in Gravitational Collapse
Model Problem: Strong Field Behaviour

- Equations of motion:

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial r}\left(\frac{\alpha}{a}\,\Pi\right) \qquad \frac{\partial \Pi}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\alpha}{a}\,\Phi\right)$$

$$\frac{1}{\alpha}\frac{d\alpha}{dr} - \frac{1}{a}\frac{da}{dr} + \frac{1-a^2}{r} = 0$$

$$\frac{1}{a}\frac{da}{dr} + \frac{a^2-1}{2r} - 2\pi r\left(\Pi^2+\Phi^2\right) = 0$$

- Total mass, M, of space-time is

$$M = m\left(\infty, t\right) \qquad a\left(r,t\right)^2 = \left(1 - \frac{2m\left(r,t\right)}{r}\right)^{-1}$$

- Coordinate system cannot penetrate interior of black holes. However, black hole formation clearly signaled in calculation by:

$$\frac{2m}{r} \to 1 \qquad \text{for some} \qquad r = R_{BH} = 2M_{BH}$$

Critical Phenomena

(MWC, *Phys. Rev. Lett.*, 1993)

- Near a critical point, the dynamics of the model problem is characterized by:
  - Exponential sensitivity to initial conditions
  - Generation of structure on arbitrarily small scales
  - "Echoing" behaviour (scale periodicity)
  - Infinitesimal black hole mass at critical point
  - Power-law scaling of black hole mass
  - Universality
  - Rapid loss of information about initial conditions

The Impact of AMR

- Berger & Oliger (1984) algorithm with minor modifications for non-hyperbolic equations: 3-level difference equations, with explicit dissipation (Kreiss & Oliger), regridding via LTE estimates

Absolutely crucial for discovery & understanding of phenomena

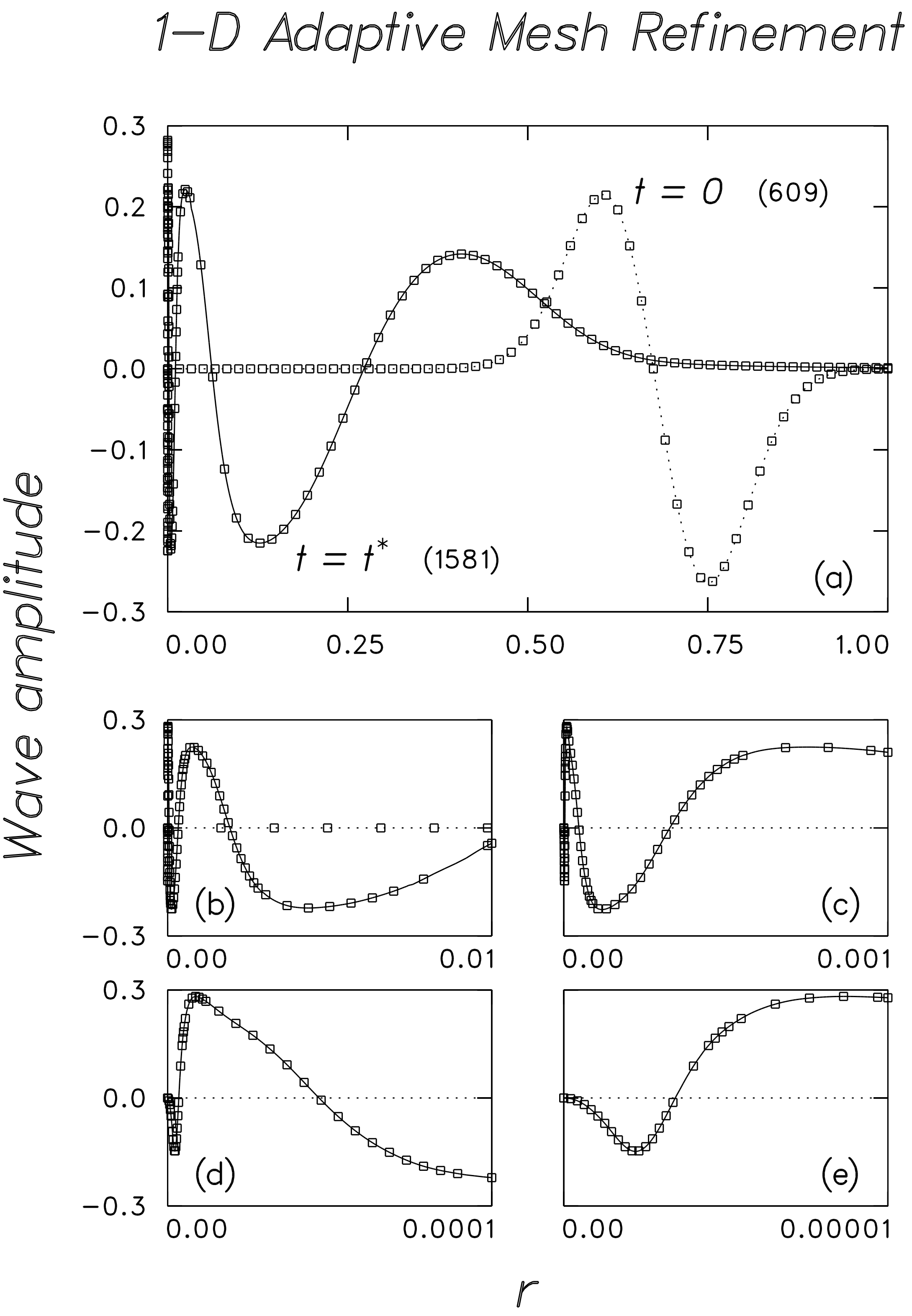
  - ◦ Generation of structure on arbitrarily small scales
  - ◦ Exponential sensitivity to initial conditions
  - ◦ Exponential sensitivity to discretization parameters near critical point: roughing out critical point at low resolution not feasible
  - ◦ Critical evolution transient in nature

- Typical run parameters: (Critical configuration)

  Coarsest grid has $\approx$ 600 points in r.
  Use 7 additional levels of 5 : 1 refinement.

  Uniform fine grid: $\approx 10^7$ spatial points; $\approx 10^{15}$ events
  In practice: ≈ 2000 spatial points; $\approx 10^7$ events

Computations almost exclusively interactive


1–D Adaptive Mesh Refinement
Wave amplitude
$t = 0$ (609)
$t = t^*$ (1581)
(a)
(b)
(c)
(d)
(e)
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
0.00
0.25
0.50
0.75
1.00
0.01
0.001
0.0001
0.00001
r

Infrastructure for (Adaptive) Parallel Computations
Motivation & Goals

- Observation: Numerical relativity codes have tended to be remarkably homogeneous from a "high-level" point of view: Almost all have employed low order (second-order) finite difference techniques on a single mesh, and have had the following structure:

```
Read (initial) state
for NUM_STEPS
  for NUM_UPDATES & maybe until convergence
    U (Grid Function(s)) -> Grid Function(s)
  end for
end for
Write (final) state
```

- Most of the hard work in developing a new code involves the construction of stable, accurate updates, U

- Also clear that significant dynamic range in black-hole problems such as binary coalescence means that adaptive-mesh-refinement (AMR) algorithms essential for efficient computation

- Ultimate goal: allow relativist to concentrate on developing stable, uni-grid code on serial architecture: parallelism and adaptivity to be "automatically" provided by the infrastructure

Infrastructure for Adaptive Parallel Computations

DAGH / GrACE

Manish Parashar (Rutgers) & J.C. Browne (UT Austin)

http://www.caip.rutgers.edu/ parashar/TASSL/

- Two main components
  - A set of programming abstractions in which computations on dynamic hierarchical grid structures are directly implementable.
  - A set of distributed dynamic data-structures that support the implementation of the of the abstractions in parallel execution environments and preserve efficient execution while providing transparent distribution of the grid hierarchy across processing elements.
- Key Features
  - Transparent access to scalable distributed dynamic Arrays, Grids, Grid-Hierarchies
  - Shadow grid-hierarchy for efficient error estimation (regridding criterion)
  - Automatic dynamic partitioning and load distribution
  - Locality in face of mutli-level data (space-filling curves).
  - Some special support for multi-grid

Infrastructure for Adaptive Parallel Computations

DAGH / GrACE 2-D Wave Example (Schematic)

```
#include "GrACE.h"
#include "GrACEIO.h"

bb[0]=xmin; bb[1]=xmax; bb[2]=ymin; bb[3]=ymax;
shape[0]=Nx; shape[1]=Ny;

GridHierarchy GH(2,NON_CELL_CENTERED,1);
GH.ACE_SetBaseGrid(bb, shape);
GH.ACE_ComposeHierarchy();
GH.ACE_IOType(ACEIO_HDF_RNPL);

BEGIN_COMPUTE

GridFunction(2)<double> phi("phi",1,1,GH,ACEComm,ACENoShadow);

for( step++; step <= nsteps; step++ ){
  forall(phi,tc,lev,c)
    update( ··· )
  end_forall
  phi.GF_Sync(tc+idt,lev,ACE_Main);
}
```

Infrastructure for Adaptive Parallel Computations

CACTUS / PUGH

Paul Walker et al (MPI Potsdam)

http://www.cactuscode.org/

- Includes PUGH package, which implements DAGH-style memory distribution/parallelization, but in a more compact C library, and only for uni-grid applications.

- Provides users of CACTUS with automatic access to parallelism.

- Code runs on essentially anything, and routinely is near or at the record for highest-sustained Gigafloppage on "realistic" problem: From http://www.ncsa.uiuc.edu/access.html

  "In June [99], the team virtually owned NCSA's 256-processor Origin2000 for a capability computing run of more than two weeks. By the time Suen and Seidel had finished their simulations, they had output nearly a terabyte of data and logged an astonishing 140,000 CPU-hours on the Origin2000."

- Significant level of support from MPI Potsdam and NSCA

The Canadian Foundation For Innovation

www.innovation.ca

(Monetary Units: 1.00 $ CAN = 0.68 $ US)

The CFI was established by the federal government with an up-front investment of $800 million. This principal amount and accrued interest will enable the Foundation to contribute, on average, about $180 million annually over five years to research infrastructure projects. The CFI targets its investment at key needs in the areas of health, environment, science, and engineering. The Foundation operates on the principle that its investments are made in partnership with the private and voluntary sectors as well as with provincial governments. The Foundation contributes 40% of total eligible project costs. On this basis, funding for the total investment by the Foundation and its partners should exceed $2 billion.

- Several programs, including *On-going New Opportunities*
  - Eligibility: First tenure track position in Canada.
  - HPC Potential at UBC from CFI: $\sim$ $1 M / yr

The `vn.physics.ubc.ca` PIII/Linux Cluster

`Doc/VN/index.html`

- 280K CFI On-going New Opps. App., 4/29/99 (UBC)
  - Affleck (Phys. & Astro.)
  - Ascher (Comp. Sc.)
  - Choptuik* (Phys. & Astro.)
  - Patey* (Chem.)
  - Salcudean* (Mech. Eng.)
  - Thachuk* (Chem.)
  - Unruh (Phys. & Astro.)

- Patterned after Chemistry machine (currently 23 compute nodes and one front-end, roughly half done), asks for
  - 64 $\times$ Dual 450 Mhz PIII/512 Mb/10 Gb (no CD ROM, keyboard, mouse, monitor) "compute nodes" 220K
  - 2 $\times$ Dual 450 Mhz PIII/512 Mb with additional peripherals "front-end nodes" 10K
  - 1 $\times$ HP-4000M Switch with 4 expansion modules $\rightarrow$ 72 (!) 100FDX ports (3.6 Gb/s back-plane) 7K
  - 13 (!) $\times$ APC Smart-UPS 1400 14K

The `vn.physics.ubc.ca` PIII/Linux Cluster

- 650K CFI On-going New Opps. App., 9/15/99 (CFI)
  - Affleck (Phys. & Astro.)
  - Ascher (Comp. Sc.)
  - Bushe* (Mech. Eng.)
  - Choptuik* (Phys. & Astro.)
  - Patey* (Chem.)
  - Salcudean* (Mech. Eng.)
  - Thachuk* (Chem.)
  - Unruh (Phys. & Astro.)
- ASKS FOR "Cluster 1" *AND*
- "Cluster 2" (focus on coarse-grained parallelism)
  - 48 $\times$ Single 600Mhz Alpha/2 Mb/256 Mb/10 Gb 230K
  - Myrinet (1000 Mb) Switch solution 32K
  - 8 $\times$ APC Smart-UPS 1400 9K
- Ultimate level of funding still somewhat unclear, but have been proceeding on the basis that we'll get something close to 650K total

The `vn.physics.ubc.ca` PIII/Linux Cluster

- 280K for vn advanced against future CFI funding 8/27
- 9/99–10/99 spent evaluating machines, finding good home, setting things up with Purchasing
- Request for bid sent out 10/7 with closing date 11/2, equipment to be delivered 16 nodes per week, with first 16 (and front ends) due 11/9, last 16 due 11/30
- Vendors: *Varsity*, *UBC Bookstore*, *AE*
- WHAT WE HAVE (last 6 compute nodes due today)

  128 (+12) 450Mhz PIIIs, 32 (+1.5) Gb RAM, 0.5 Tb disk

  - 64 compute: 2 x 450Mhz PIII/512 Mb/10 Gb IDE 180k
  - 3 front-ends: 2 x 450Mhz PIII/512 Mb/34 Gb SCSI 20K
  - 1 $\times$ HP-4000M Switch: 7K
  - 4 $\times$ APC Matrix 3000M with 8 PDUs: 19K
- Estimated total expenditures: 250K

The `vn.physics.ubc.ca` PIII/Linux Cluster

- Assembly & Software Installation Team
  - Jason Ventrella
  - Inaki Olabarrieta
  - Choptuik
  - Unruh
- At vendor (3747 W 10th, Vancouver)
  - BIOS settings
  - "Everything" (!) install of Mandrake 6.1 at vendor's site
  - Network configuration including IP address assignment
- At our site (Main Machine Room, Old CS Bldg, UBC)
  - Plug node in, attach to network, power up
  - Secondary software installation
- On node `N` hardware failure (5 or 6 so far)
  - Swap identities of `vnN` and `vnNMAX` (either via disk swap or software), send `vnNMAX` to Varsity.
  - Decrement `vnNMAX` and update system files.

vn.physics.ubc.ca: First 16 compute nodes & 3 front-ends

vn.physics.ubc.ca: Back-end View

The `vn.physics.ubc.ca` PIII/Linux Cluster

Applications Run to Date

- "shell-level" parallelism
  - Ethan Honda (UT Austin grad stud): detailed parameter space survey of "oscillons" (typically 40 + processes)
  - Roman Petryk (UBC grad stud): quantum gravity inspired calculations (typically 40 + processes)

- MPI-based parallelism
  - Luis Lehner (UT Austin postdoc), Mijan Huq (Penn State RA): 3D black hole calculations
    (81 x 81 x 81 spends 11% in communications. Could do 161 x 161 x 161)
  - Lothar Buchmann, TRIUMF Research Scientist: Nuclear physics.
  - Roman Baranowski, UBC Chemistry postdoc (??)

MANY MORE TO COME!

The vn.physics.ubc.ca PIII/Linux Cluster

The anarchy queueing system

```
vnfe1 % ruptime | grep -v down | grep -v vnfe | sort -n +6

vn10 up 9+11:34, 0 users, load 0.00, 0.00, 0.00
vn11 up 9+11:34, 0 users, load 0.00, 0.00, 0.00
vn13 up 9+11:34, 0 users, load 0.00, 0.00, 0.00
vn15 up 9+11:31, 0 users, load 0.00, 0.00, 0.00
vn20 up 9+11:32, 0 users, load 0.00, 0.00, 0.00
vn21 up 9+11:32, 0 users, load 0.00, 0.00, 0.00
vn22 up 9+11:32, 0 users, load 0.00, 0.00, 0.00
vn23 up 9+11:28, 0 users, load 0.00, 0.00, 0.00
vn24 up 9+11:28, 0 users, load 0.00, 0.00, 0.00
vn26 up 9+11:29, 0 users, load 0.00, 0.00, 0.00
vn35 up 9+11:27, 0 users, load 0.00, 0.00, 0.00
vn39 up 9+11:27, 0 users, load 0.00, 0.00, 0.00
vn40 up 9+11:28, 0 users, load 0.00, 0.00, 0.00
vn41 up 9+11:28, 0 users, load 0.00, 0.00, 0.00
vn42 up 9+11:28, 0 users, load 0.00, 0.00, 0.00
vn43 up 4+01:51, 0 users, load 0.00, 0.00, 0.00
vn44 up 4+22:16, 0 users, load 0.00, 0.00, 0.00
vn8 up 9+11:34, 0 users, load 0.00, 0.00, 0.00
vn9 up 9+11:34, 0 users, load 0.00, 0.00, 0.00
vn33 up 9+11:26, 0 users, load 0.97, 0.91, 0.82
vn38 up 8+17:48, 0 users, load 1.82, 1.91, 1.89
                         .
                         .
                         .
vn53 up 4+21:31, 0 users, load 2.27, 2.20, 2.08
```