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
SCV Seminar, UBC, November 29, 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:

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

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

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

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 $\equiv$ Laser Interferometer Gravitational-Wave Observatory

- Some Vital Statistics
  - Interferometer arms: 4 km
  - Sensitivity band: $\approx$ 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)

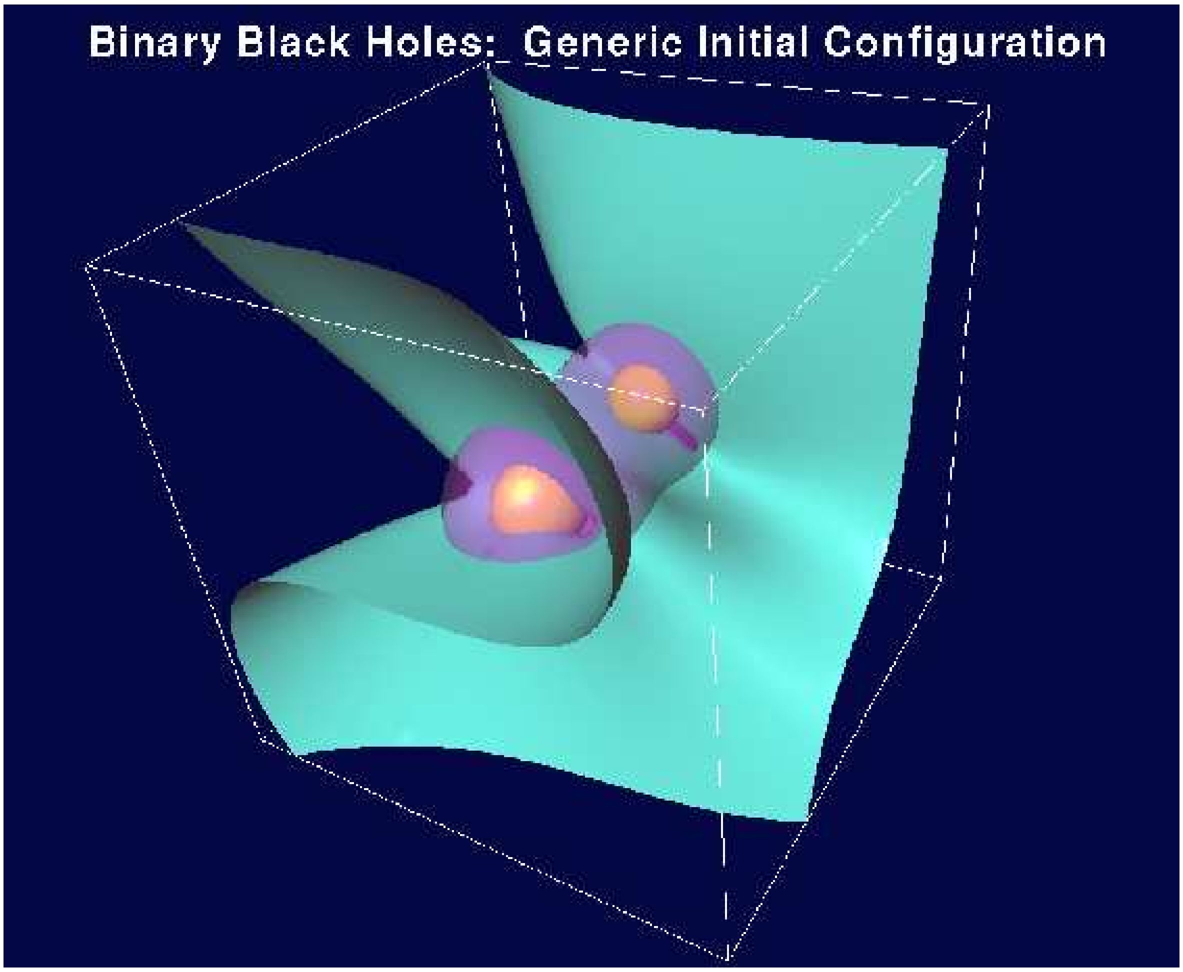
$$\mathcal{F}_\mu[\alpha, \beta^i; g_{ij}, K_{ij}] = 0$$

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

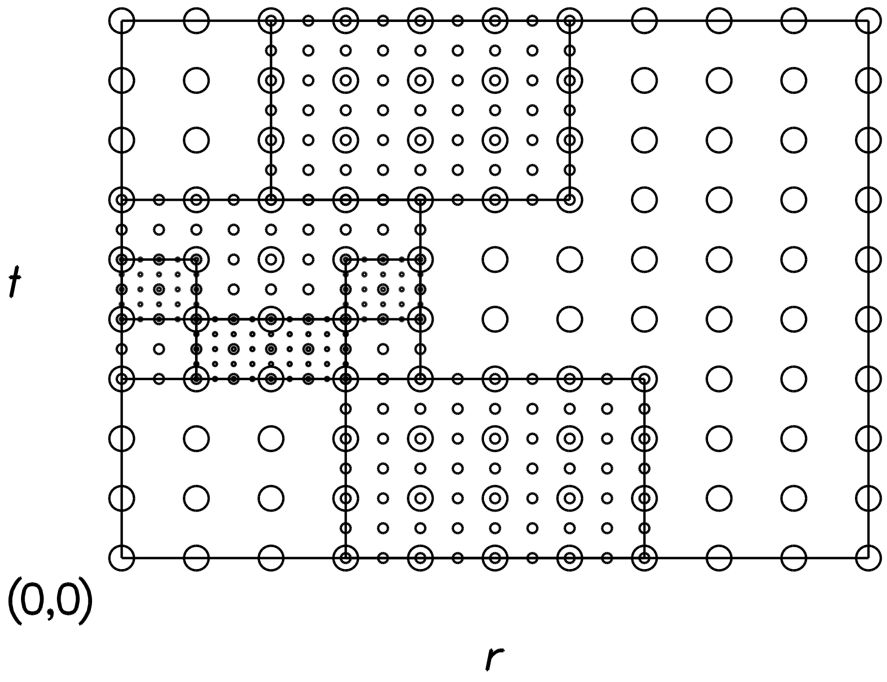
- Typical black hole problem requires significant dynamical range

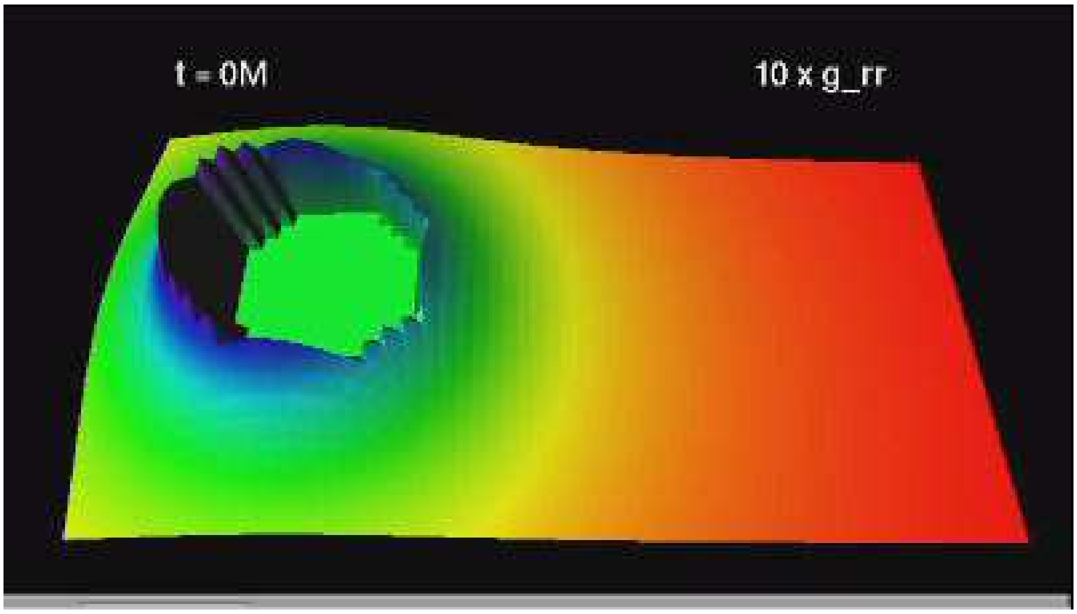
$$\lambda_{\mathrm{radiation}} \sim 100\, R_{\mathrm{BH}}$$

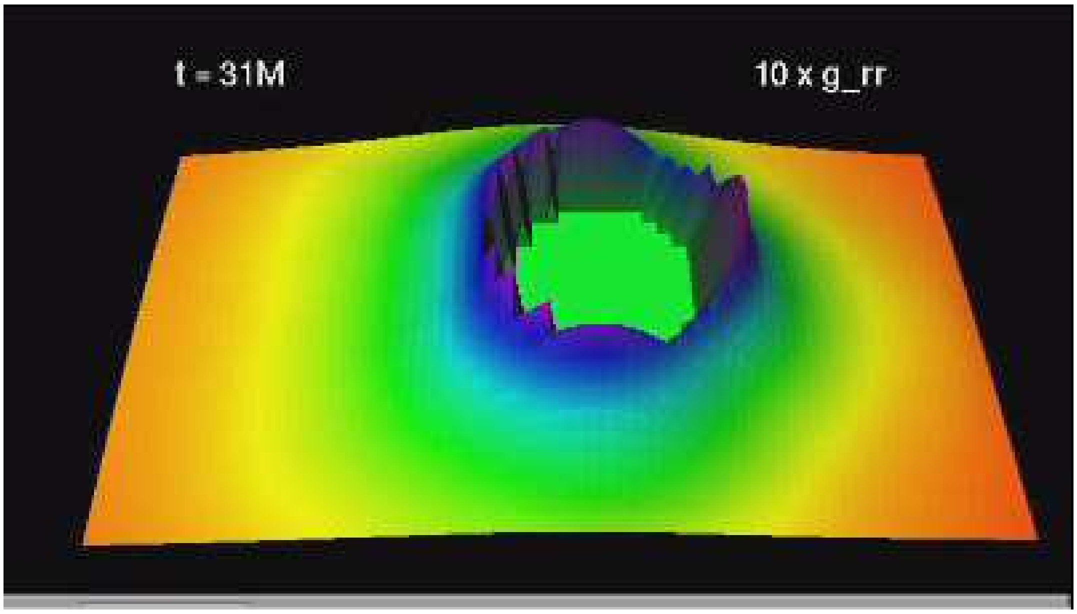
- Some form of adaptive mesh refinement will be crucial for efficient 3-D computations
- Strategy: Implement *some* sufficient algorithm, don't worry if it isn't optimally efficient as long as scaling of computational time with "physical process" is roughly linear.
- "Minimal" Berger & Oliger algorithm (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

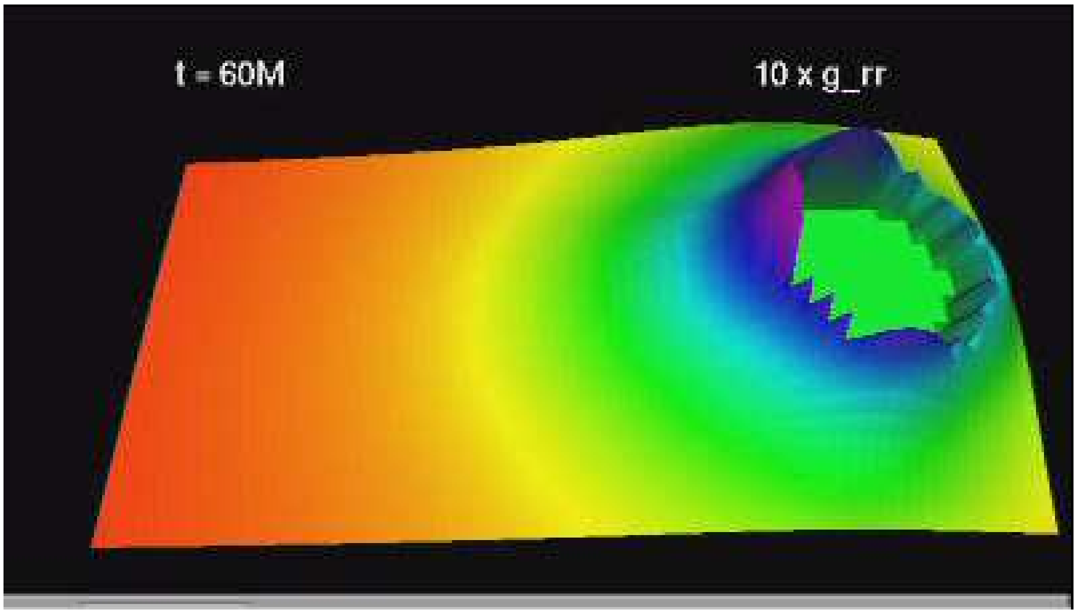
Schematic Adaptive–Mesh Structure

2 : 1 Refinement in Space and Time



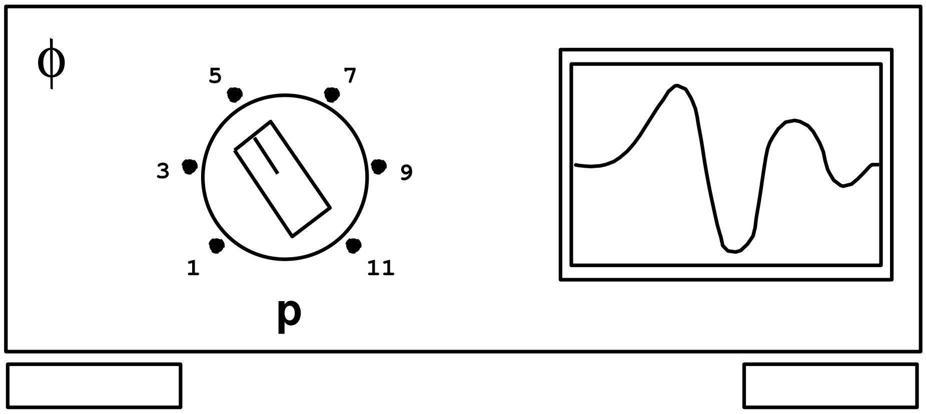

t = 0M
10 x g_rr


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

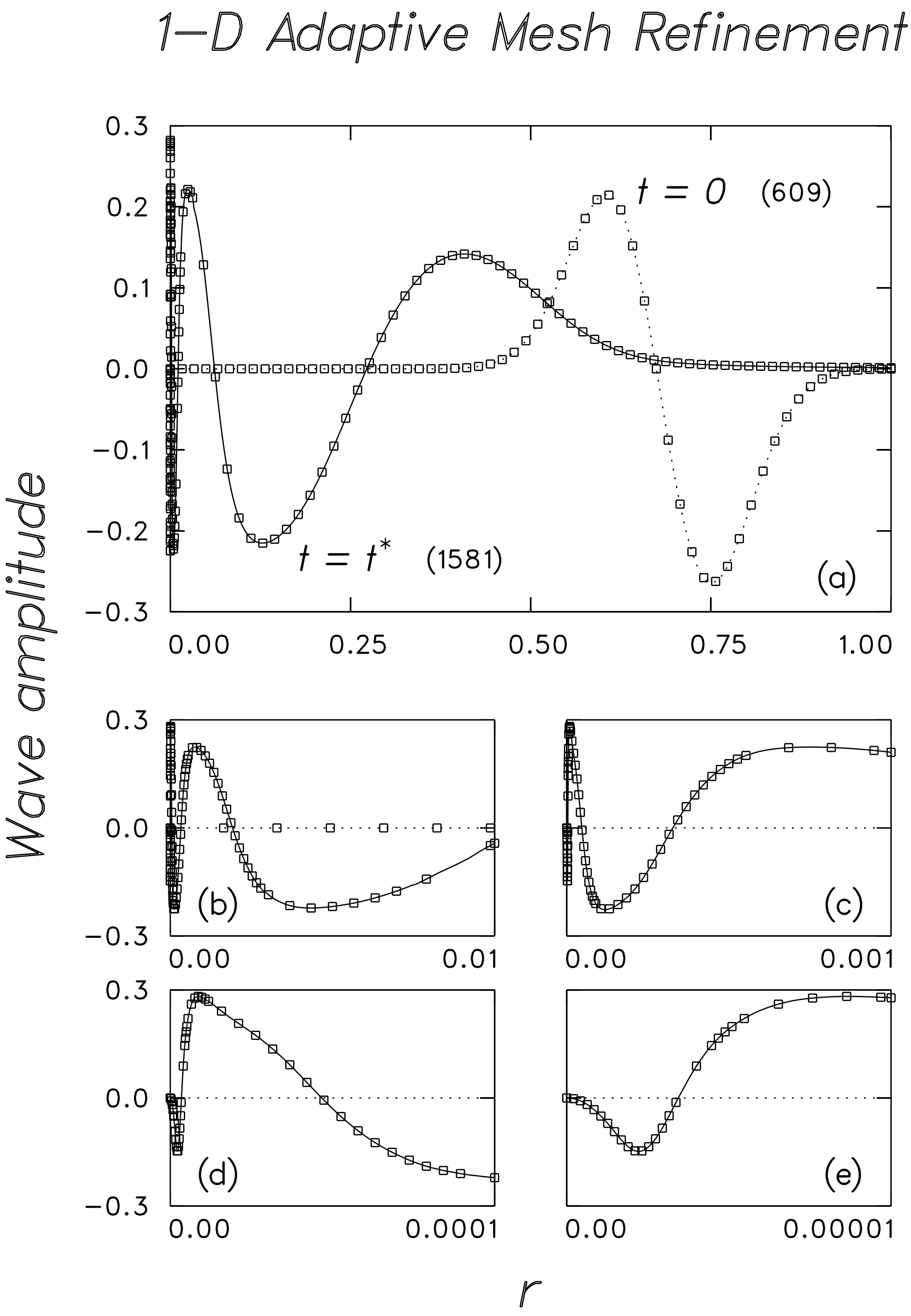
  - Generation of structure on arbitrarily small scales
  - Exponential sensitivity to initial conditions
  - Exponential sensitivity to discretization parameters near critical point: roughing out critical point at low resolution not feasible
  - Critical evolution transient in nature

- 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
r
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

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

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 vn.physics.ubc.ca PIII/Linux Cluster

Doc/VN/index.html

- 280K CFI On-going New Opps. App., 4/29/99 (UBC)
  Doc/CFI.april99/index.html
  - Affleck (Phys. & Astro.)
  - Ascher (Comp. Sc.)
  - Choptuik⋆ (Phys. & Astro.)
  - Patey⋆ (Chem.)
  - Salcudean⋆ (Mech. Eng.)
  - Thachuk⋆ (Chem.)
  - Unruh (Phys. & Astro.)

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

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

- 650K CFI On-going New Opps. App., 9/15/99 (CFI)
  `Doc/CFI/index.html`
  - 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

- Comparison with zodiac.chem.ubc.ca (**zd**)
  - **zd** compute node: 2 x 450 Mhz PIII 256 Mb/4 Gb IDE
  - **vn** compute node: " " " 512 Mb/12 Gb IDE
  - **zd**: 1 front-end: 2 x 450 Mhz PIII 512 Mb/20 Gb SCSI
  - **vn**: 3 front-ends: " " " 512 Mb/34 Gb SCSI
  - **vn**: 3 DATS (SCSI)
  - **zd**: 1 DAT (SCSI)
  - **zd**: Running in custom-built security caging in air-conditioned, power-reconditioned room in Chemistry.
  - **vn**: Running in secure machine room in Klinck (Old CS), so far have paid 6K for back-bone, 1K for electrical, will pay 7K annual "rent"; 2-yr agreement starts tomorrow
  - **zd**: Connect to/from "outside-world" via front-end only.
  - **vn:** Connect to/from "outside-world" via any node.
  - **zd** currently running DQS queueing system.
  - **vn** currently running anarchy :-) queueing system.

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

- Assembly & Software Installation Team
  - Jason Ventrella
  - Inaki Olabarrieta
  - Choptuik
  - Unruh
- At vendor (3747 W 10th)
  - BIOS settings
  - "Everything" (!) install of Mandrake 6.1 at vendor's site
  - Network configuration including IP address assignment
- At our site (Klinck Building)
  - 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
  - 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
```