Software for Solving Elliptic PDEs With Parallel Adaptive Multi-level Methods

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The Changing Face of Mathematical Software

PHAML

- Parallel Hierarchical Adaptive Multi-Level
- Fortran 90 program
- 2D Elliptic PDE solver (BVP and eigenvalue)
- Adaptive finite elements with multigrid
- Message passing parallelism: MPI or PVM
- Optional: Zoltan, OpenGL, ARPACK, PetSC, hypre, MUMPS, SuperLU

Outline

- Computational Setting
- Numerical Methods
- Software Design
- User Interface
- Graphics
- Conclusion

Elliptic Boundary Value Problems

$$
\begin{aligned}
-\frac{\partial}{\partial x}p\frac{\partial u}{\partial x} - \frac{\partial}{\partial y}q\frac{\partial u}{\partial y} + ru &= f \quad \text{in } \Omega \subset \Re^2 \\
u &= g_1 \text{ on } \partial\Omega_1 \\
\frac{\partial u}{\partial n} + cu &= g_2 \text{ on } \partial\Omega_2
\end{aligned}
$$

p, q, r, f, c, g_1 and g_2 functions of (x, y)
$\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$
Ω polygonal

Also: time dependent, nonlinear, systems

Elliptic Eigenvalue Problems

$$\begin{aligned}
-\frac{\partial}{\partial x} p \frac{\partial u}{\partial x} - \frac{\partial}{\partial y} q \frac{\partial u}{\partial y} + ru &= \lambda u \ \text{ in } \ \Omega \subset \Re^2 \\
u &= 0 \quad \text{ on } \ \partial\Omega_1 \\
\frac{\partial u}{\partial n} &= 0 \quad \text{ on } \ \partial\Omega_2
\end{aligned}$$

p, q, r functions of (x, y)

$\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$

Ω polygonal, generally a truncation of an infinite domain

Computational Environment

- Network of workstations or PCs
  - modest number of processors (10's)
  - distributed memory parallelism with message passing
  - now a common parallel computer in resource-limited labs
- vs. expensive massively parallel machines
  - smaller bandwidth
  - much higher latency
  - need parallel algorithms with infrequent messages

Numerical Methods

- Parallelization of methods in MGGHAT
- Standard finite elements, linear, triangles
- Newest node bisection adaptive refinement
- Hierarchical basis multigrid
- Refinement-tree based grid partitioning
- Full domain partition

Adaptive Multilevel Algorithm

start with very coarse mesh

repeat

    if the load is too far out of balance

        repartition grid

        redistribute data

    endif

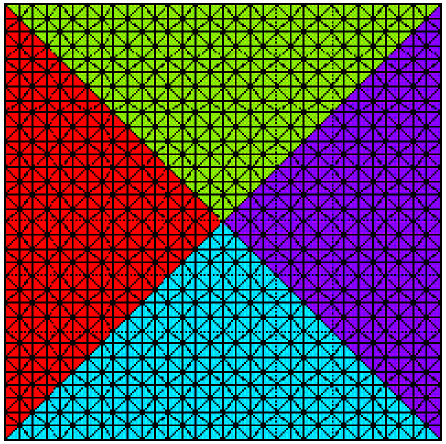
    adaptive mesh refinement

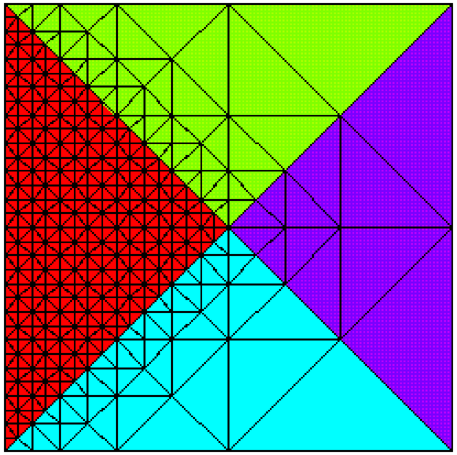
    multigrid cycles

until termination criterion is met

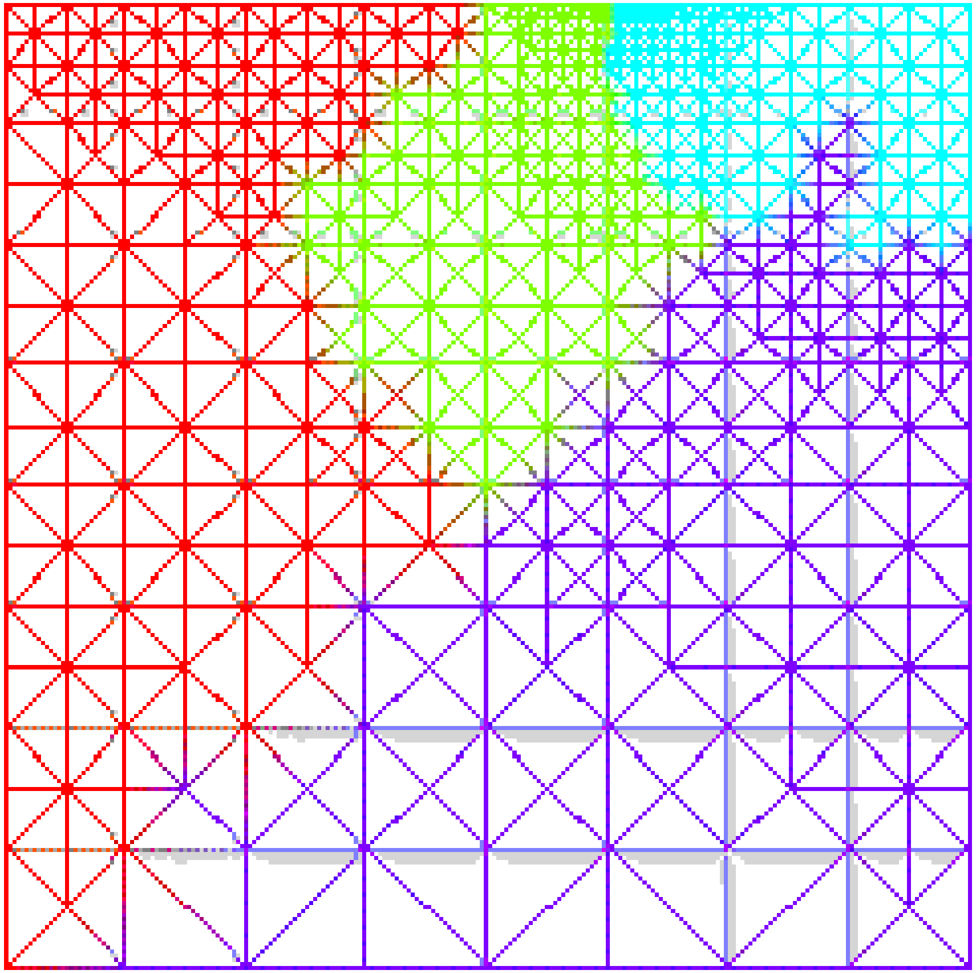
Full Domain Partition

- Each processor gets the triangles from a partition
- Each processor receives additional shadow data
  - just enough to cover the full domain
  - taken from coarser refinement levels
  - $O(\sqrt{N})$ extra data

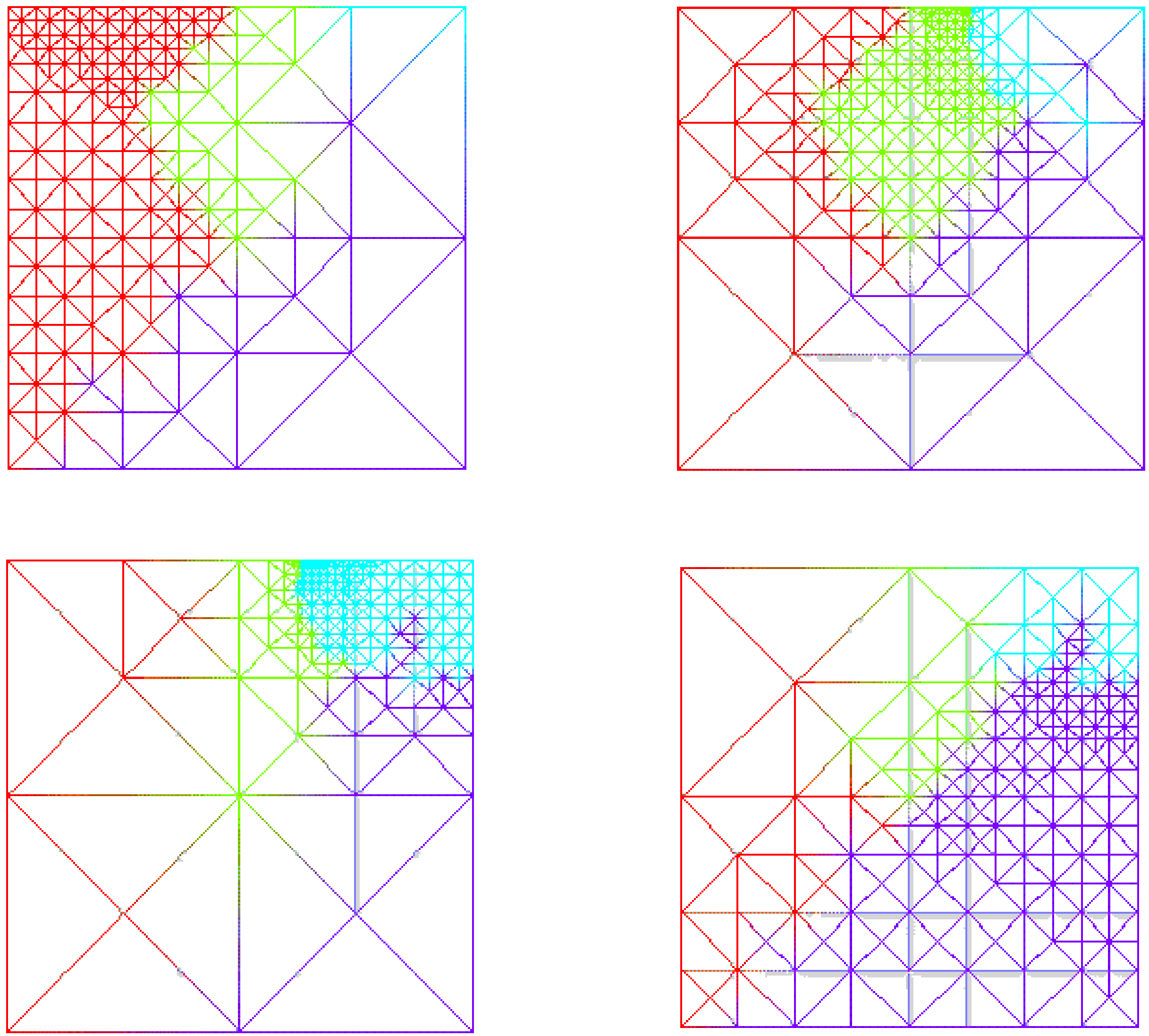




Full Domain Partition Example



Full Domain Partition Example



Grid Partitioning

- Goal: balance the load, minimize communication
- Must be very fast
- Must work on distributed data
- Zoltan library (Devine et al., Sandia)
  - recursive coordinate and inertial bisection
  - space filling curve methods
  - refinement-tree based method
  - ParMetis, Jostle

Refinement-tree Based Method

- Refinement tree
  - nodes correspond to elements
  - children of a node are elements created by refinement
- Label the leaves with a weight
- Traverse the tree to compute subtree weights
  - the only communication occurs during this step
- Traverse the tree to assign subtrees to a partition until the partition contains *(total weight)/p*
- Achieves perfect balance, contiguous partitions

Adaptive Refinement

- Goal is to concentrate the effort where it does the most good
- Estimate the error on each element and refine those with the largest error estimate
- Many methods for:
  - error estimate
  - element refinement
  - maintaining compatibility
  - when to quit

Parallel Adaptive Refinement

- Refine each partition independently, but only refine *owned* triangles with large error estimate and triangles for compatibility
- Send a list of unowned triangles that were refined to the other processors
- Refine owned triangles that other processors refined
- Enforce overlap requirements

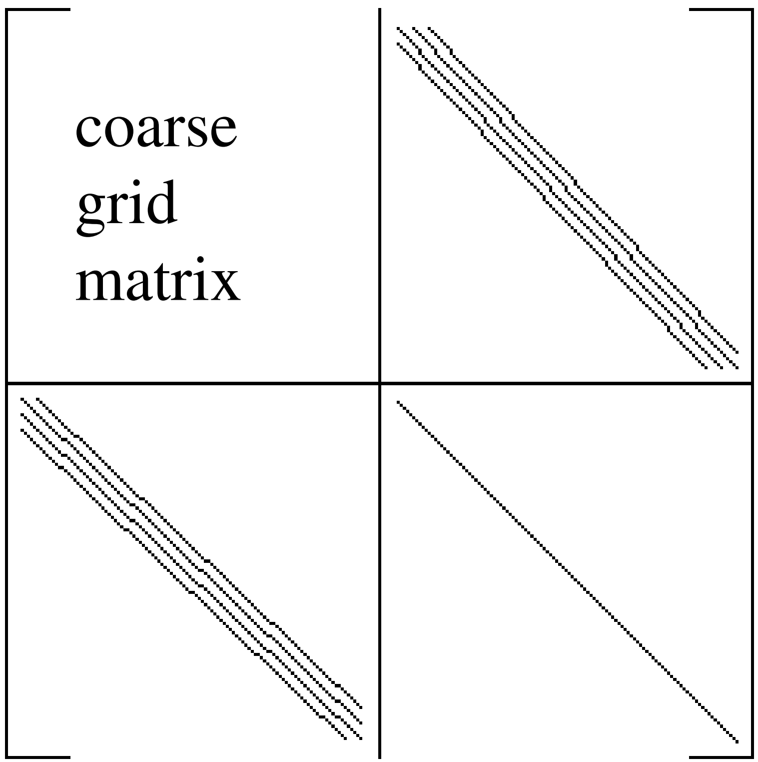
Multigrid

- Use a sequence of grids to solve in O(N) operations
  - Smooth error on current grid (e.g. Gauss-Siedel)
    - Reduces high frequency components of error
  - Define and solve a problem on a coarser grid
    - Lower frequency components are high frequency here
    - Recursively apply procedure
  - Use coarse grid solution to correct fine grid solution
  - Smooth again on fine grid
- For a large class of PDEs, reduces the error by a contraction factor independent of N

Hierarchical Multigrid

coarse level nodes

finest level nodes



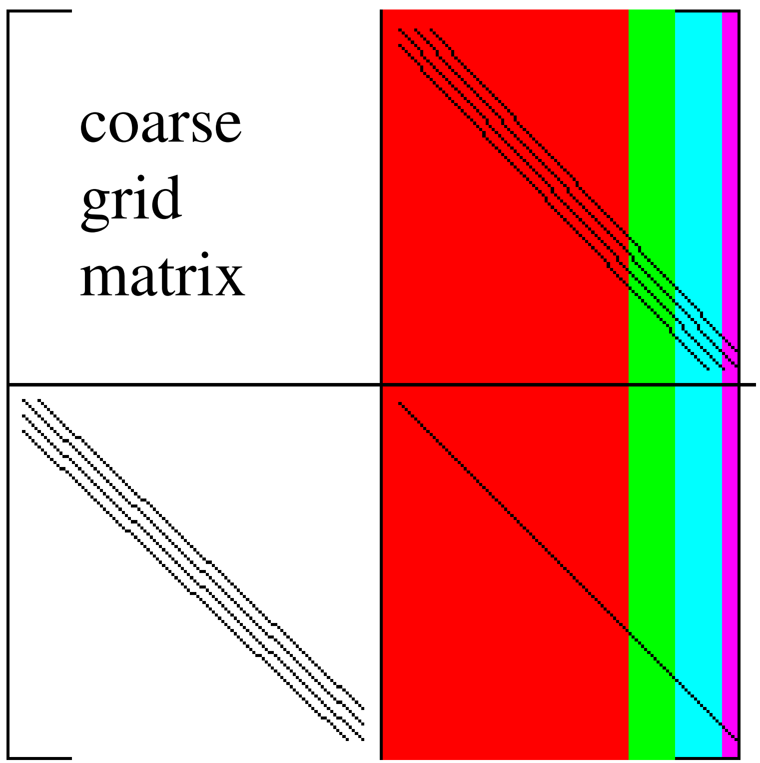
$$= \begin{bmatrix} A_c & A^T_{cf} \\ A_{cf} & A_f \end{bmatrix}$$

$$A_c x_c = b_c - A^T_{cf} x_f$$

Parallel Hierarchical Multigrid

coarse level nodes

finest level nodes



$$= \begin{bmatrix} A_c & A^T_{cf} \\ A_{cf} & A_f \end{bmatrix}$$

$$A_c x_c = b_c - {\color{red}A^T_{cf} x_f} - {\color{green}A^T_{cf} x_f} - {\color{cyan}A^T_{cf} x_f} - {\color{magenta}A^T_{cf} x_f}$$

Parallel Hierarchical Multigrid

downward part of cycle

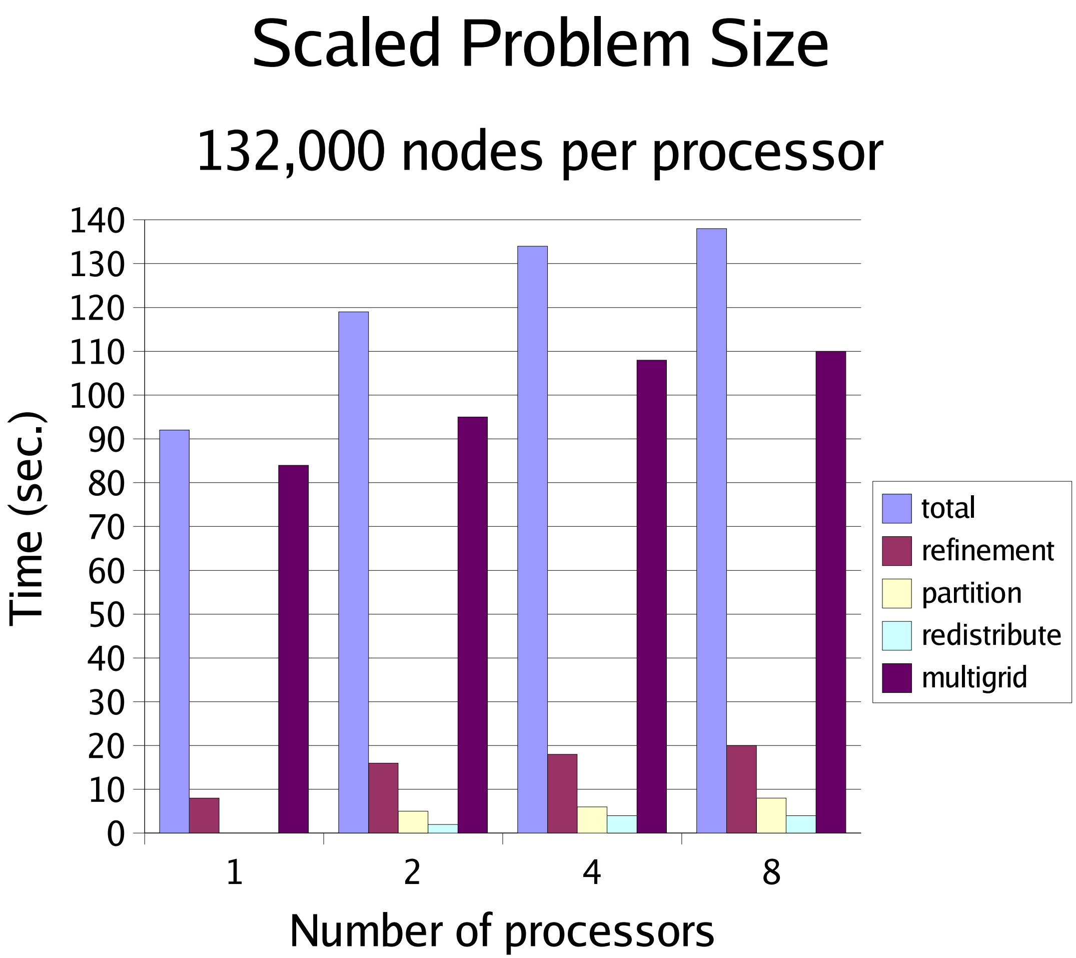
send new solution and $A^T_{cf} x_f$ to other processors

solve on coarsest grid

upward part of cycle

send new solution to other processors

Parallel Efficiency



Efficiency

Refinement	50%
Multigrid	75%
Overall	66%

Fortran 90 Modules

- Contain variables, constants, type definitions, etc.
- Entities can be public or private
- Use for
  - Global data
  - Library interface definition
  - Data encapsulation
  - Many other uses

Data Encapsulation

- Public type with private internals
- Operations on that type
- PHAML has two forms of hash_key

```
public hash_key, hash_insert, hash_remove

type hash_key
   private
   integer :: key
end type hash_key
```

Primary PHAML Modules

- phaml
- grid, grid_type
- linear_system and subordinates
- load_balance
- message_passing
- hash, sort
- graphics
- global
- interfaces to other software packages

Data Structures

```
type phaml_solution_type
   private
   type(grid_type) :: grid
   type(proc_info) :: procs
   integer :: outunit, errunit, pde_id
   character(len=HOSTLEN) :: graphics_host
   logical :: i_draw_grid, master_draws_grid, &
              still_sequential
end type phaml_solution_type
```

Data Structures

```
type grid_type
   type(element_type), pointer :: element(:)
   type(node_type), pointer :: node(:)
   type(hash_table) :: elem_hash, node_hash
   integer :: next_free_elem, next_free_node
   integer, pointer :: head_level_elem(:), &
                       head_level_node(:)
   integer :: partition
   integer :: nelem, nelem_leaf, nelem_leaf_own, &
              nnode, nnode_own, nlev
end type grid_type
```

Data Structures

```
type node_type
   type(hash_key) :: gid
   type(point) :: coord
   real :: solution
   integer :: type, assoc_elem, next, previous
end type node_type
```

User Interface

- User written external subroutines
  - **`pdecoefs, bconds, iconds, trues, true_energies_sq, init_grid, integral_kernel`**
- Public PHAML subroutines
  - **`create, destroy, solve_pde, evaluate, query, integrate, connect, store, restore, popen, pclose`**
- Main program that uses the PHAML library

User Written Subroutines

```
subroutine pdecoefs(x,y,cxx,cyy,c,rs)

! pde is
! -( cxx(x,y)*u ) -( cyy(x,y)*u ) +c(x,y)*u = rs(x,y)
!               x x              y y

real, intent(in) :: x, y
real, intent(out) :: cxx(:,:),cyy(:,:),c(:,:),rs(:)

cxx(1,1) = 1.0
cyy(1,1) = 1.0
c(1,1)   = 0.0
rs(1)    = x*x + y*y

end subroutine pdecoefs
```

Public PHAML Subroutines

- Operate on **`phaml_solution_type`** variables
- Optional arguments
  - Simplify calling sequences
  - Reasonable defaults for missing arguments
    - Some arguments useful only to experts
  - Help upward compatibility

Arguments for solve_pde

```
subroutine solve_pde(phaml_solution, iterm,                         &
           max_elem, max_node, max_lev, max_refsolveloop,           &
           init_form, comm_freq, partition_size, eq_type,           &
           print_grid_when, print_grid_who, print_error_when,       &
           print_error_who, print_time_when, print_time_who,        &
           print_eval_when, print_eval_who,                         &
           print_header_who, print_trailer_who, clocks,             &
           draw_grid_when, draw_reftree_when, pause_after_draw,     &
           pause_after_phases, pause_at_start, pause_at_end,        &
           uniform, overlap, sequential_node, inc_factor,           &
           error_estimator, refterm, derefine,                      &
           partition_method, predictive,                            &
           solver, preconditioner, mg_cycles, mg_prerelax,          &
           mg_postrelax, iterations, ignore_quad_err,               &
           final_solves, final_mg_cycles,                           &
           num_eval, lambda0)
```

Example `main` Program

```
program user_main_example
use phaml
type(phaml_solution_type) :: pde
call create(pde, draw_grid_who = MASTER)
call solve_pde(pde,                                  &
               max_node = 20000,                     &
               draw_grid_when = PHASES,              &
               partition_method = ZOLTAN_RCB,        &
               mg_cycles = 2)
call destroy(pde)
end program
```

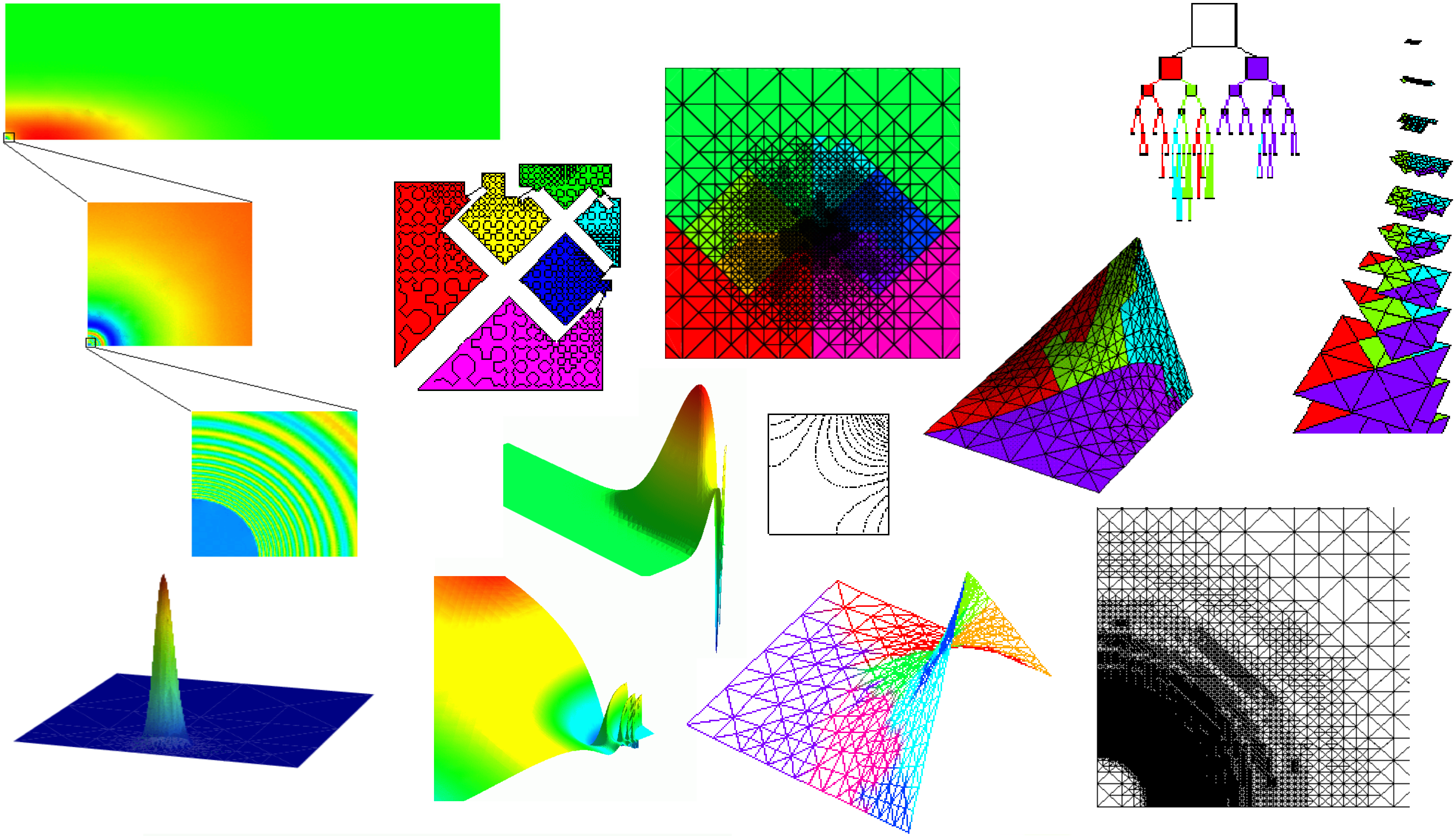
Parallelism

- Distributed memory computers
  - DM parallel computers, e.g. SP2
  - Clusters
- Message passing
  - MPI, PVM
- Parallel modes
  - Spawning: master/slave/graphics
  - Spawnless: SPMD
  - Sequential

Parallelism

- Four versions of module **`message_passing`**
  - All communication goes through this module
- Parallelism is hidden
  - User provides main program only for master
- Consider slaves/graphics as part of a **`phaml_solution_type`** object
  - Parallel config hidden in component **`proc_info`**
  - Processes spawned by subroutine create
  - Processes killed by subroutine destroy

Graphics



Conclusion

- PHAML is a new elliptic PDE solver
- Parallel sequel to MGGHAT
- Adaptive refinement, multigrid, message passing
- Fortran 90 improves code quality, user interface
- Tested on several unixes, compilers
- PHAML is in the public domain
  - http://math.nist.gov/phaml
  - william.mitchell@nist.gov