Scalable Visual Comparison of Biological Trees and Sequences

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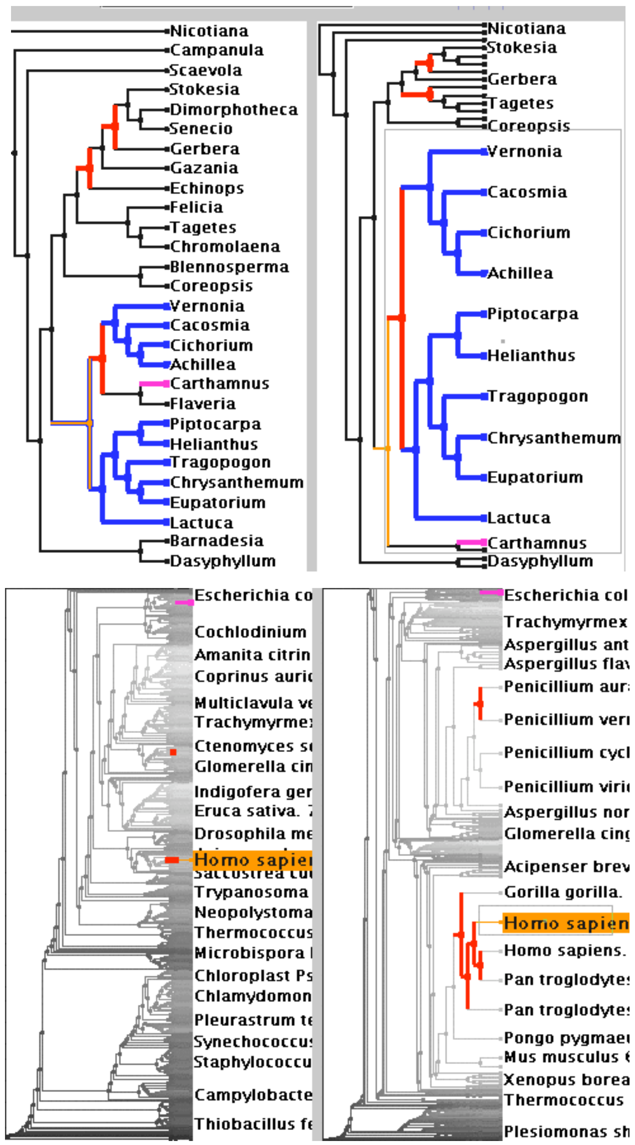
Imager

Outline

- Accordion Drawing
  - information visualization technique
- TreeJuxtaposer
  - tree comparison
- SequenceJuxtaposer
  - sequence comparison
- PRISAD
  - generic accordion drawing framework

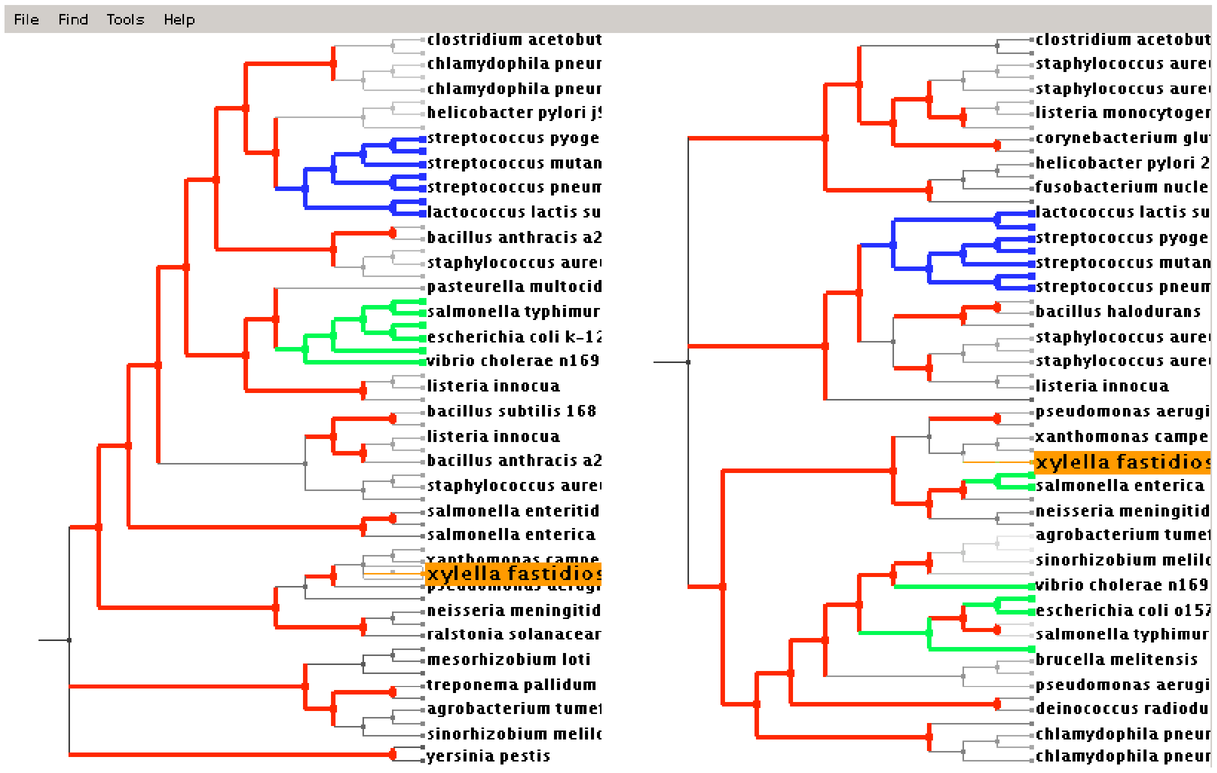
Accordion Drawing

- rubber-sheet navigation
  - stretch out part of surface, the rest squishes
  - borders nailed down
  - Focus+Context technique
    - integrated overview, details
  - old idea
    - [Sarkar et al 93], [Robertson et al 91]
- guaranteed visibility
  - marks always visible
  - important for scalability
  - new idea
    - [Munzner et al 03]

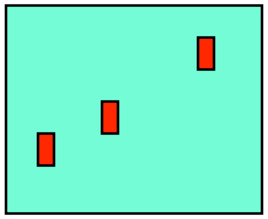


Guaranteed Visibility

- marks are always visible
- easy with small datasets



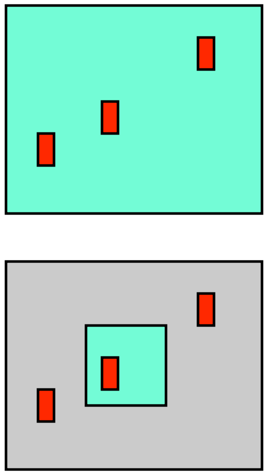
Guaranteed Visibility Challenges



- hard with larger datasets
- reasons a mark could be invisible

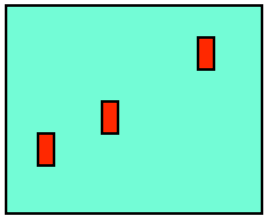
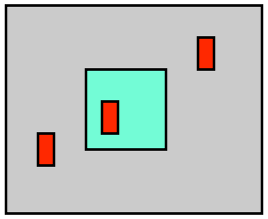
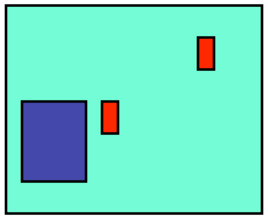
Guaranteed Visibility Challenges

- hard with larger datasets
- reasons a mark could be invisible
  - outside the window
    - AD solution: constrained navigation



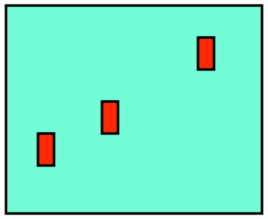
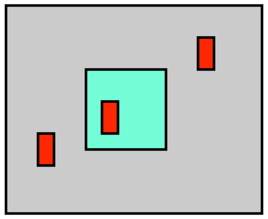
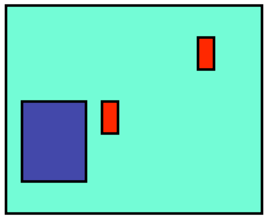
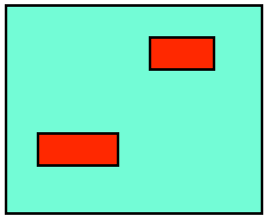
Guaranteed Visibility Challenges

- hard with larger datasets
- reasons a mark could be invisible
  - outside the window
    - AD solution: constrained navigation
  - underneath other marks
    - AD solution: avoid 3D

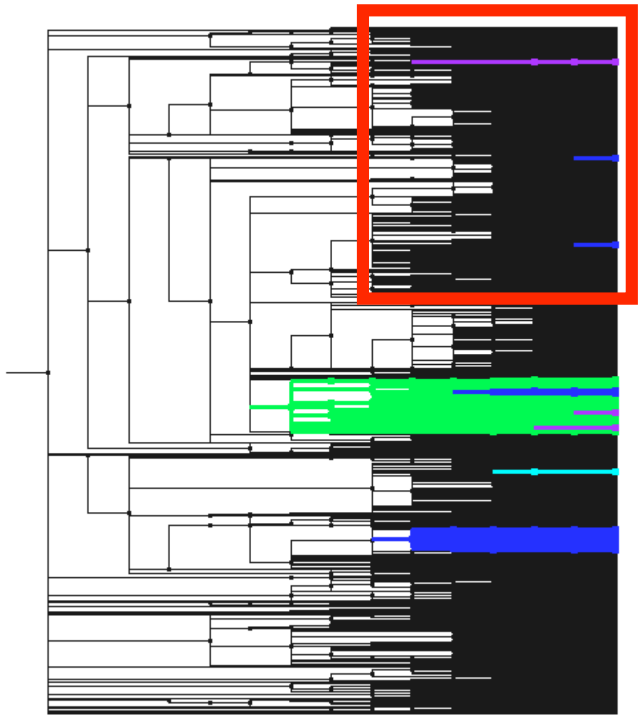
Guaranteed Visibility Challenges

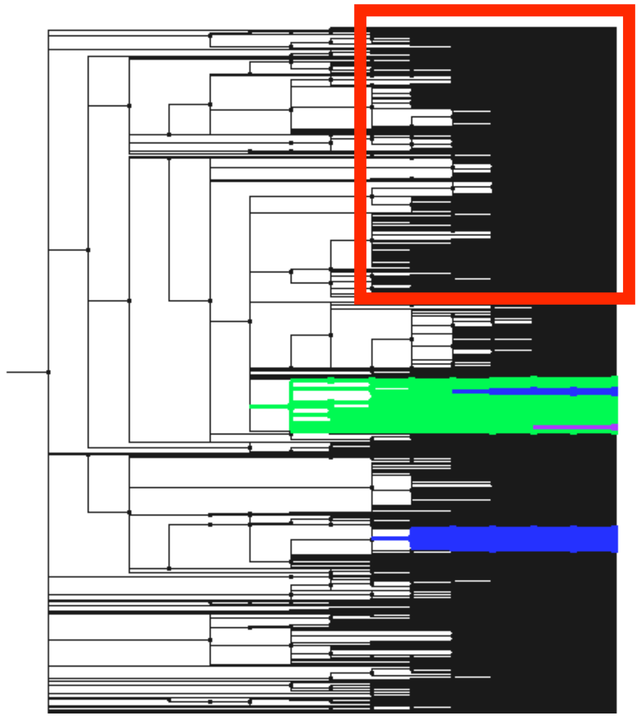
- hard with larger datasets
- reasons a mark could be invisible
  - outside the window
    - AD solution: constrained navigation
  - underneath other marks
    - AD solution: avoid 3D
  - smaller than a pixel
    - AD solution: smart culling

Guaranteed Visibility: Small Items

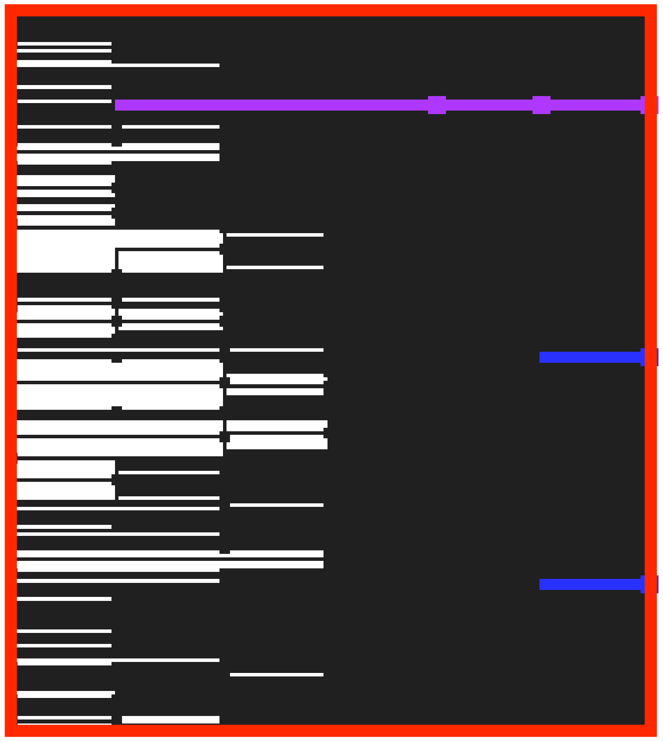
- Naïve culling may not draw all marked items


Guaranteed visibility of marks

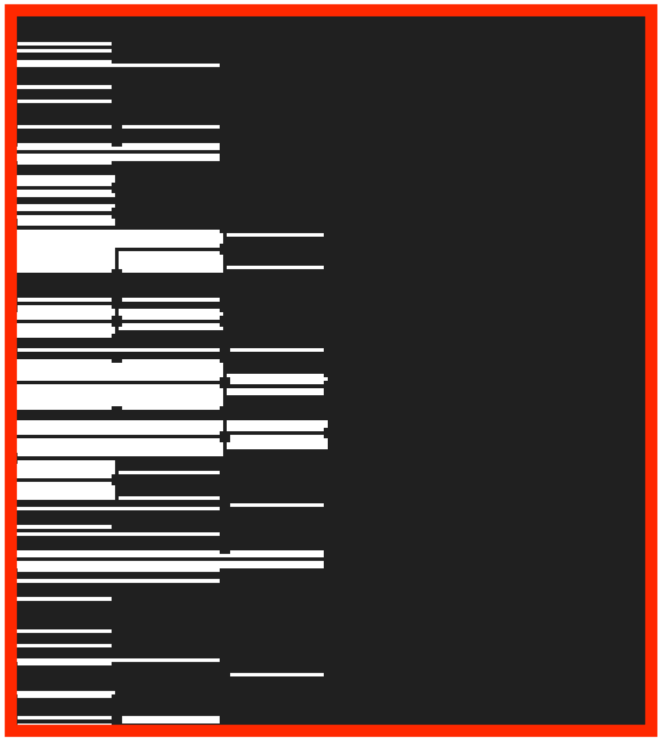

No guaranteed visibility

Guaranteed Visibility: Small Items

- Naïve culling may not draw all marked items



Guaranteed visibility of marks



No guaranteed visibility

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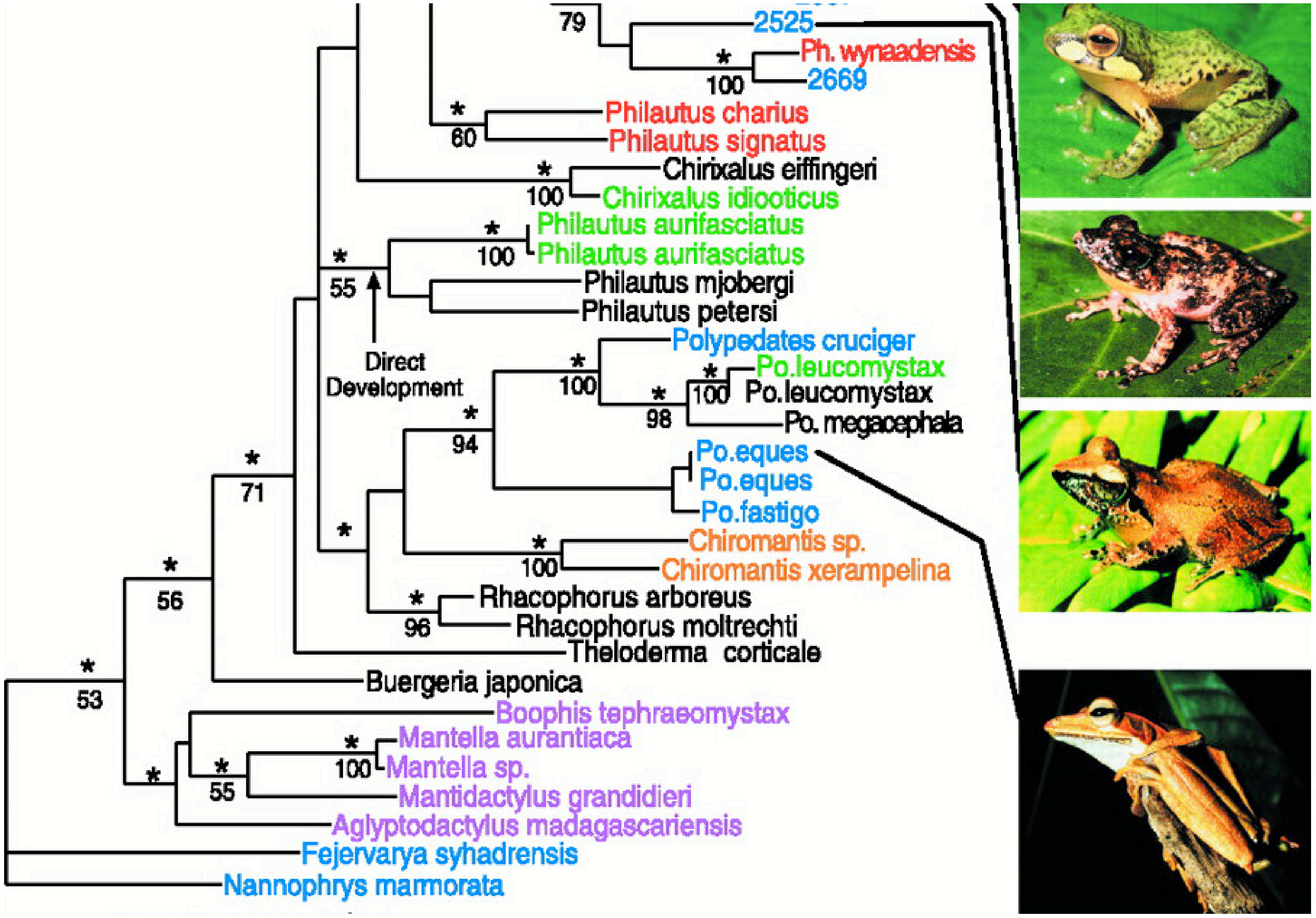
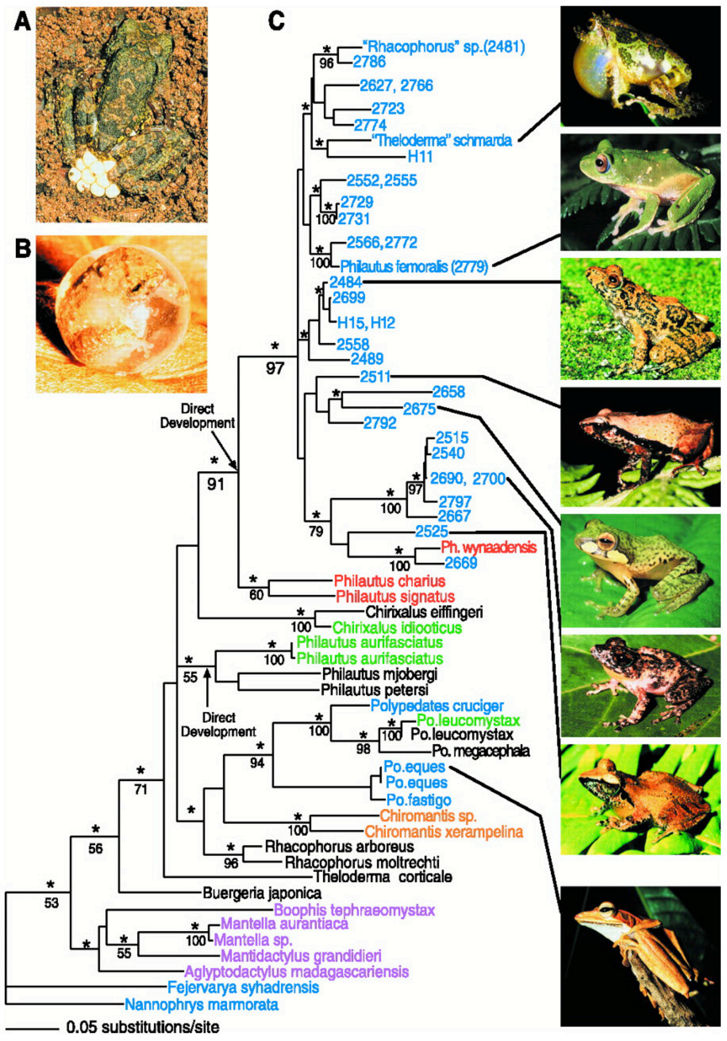
Phylogenetic/Evolutionary Tree



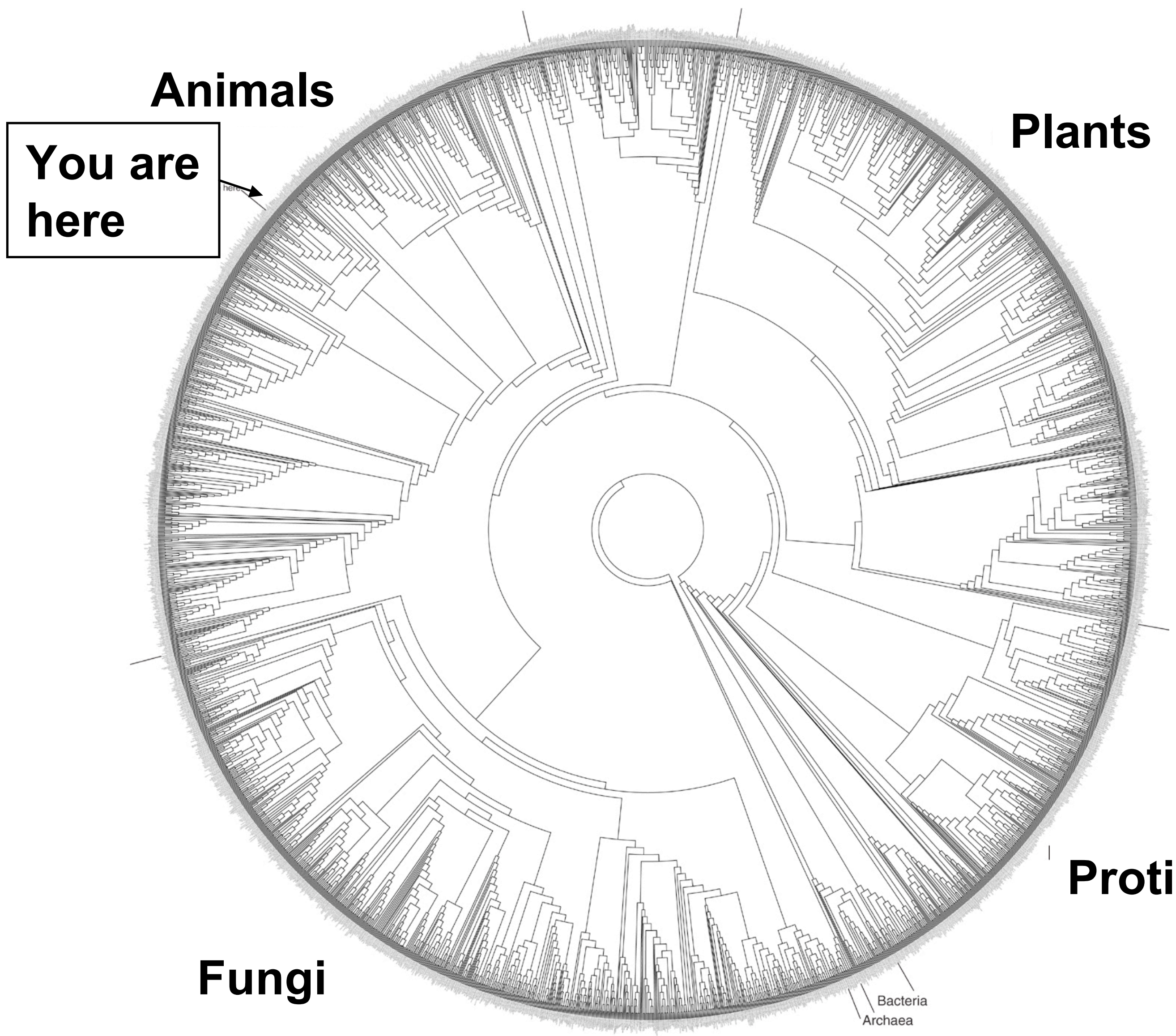
M Meegaskumbura et al., Science 298:379 (2002)

Common Dataset Size Today



M Meegaskumbura et al., Science 298:379 (2002)

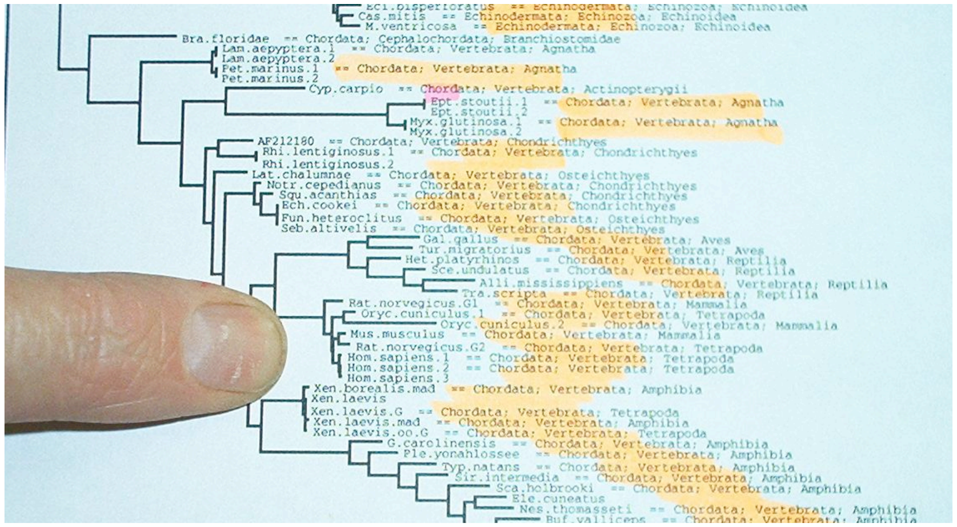
Future Goal: 10M node Tree of Life



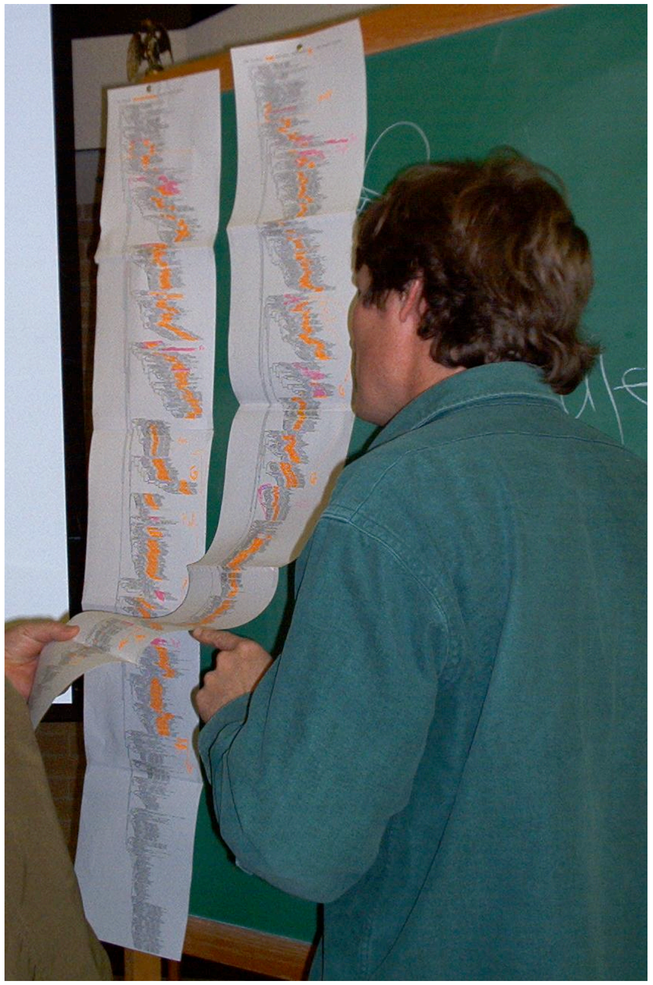
David Hillis, Science 300:1687 (2003)

Paper Comparison: Multiple Trees

focus

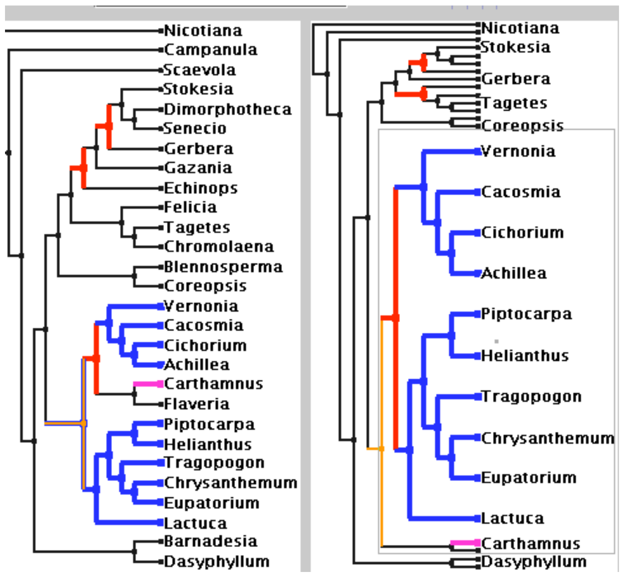


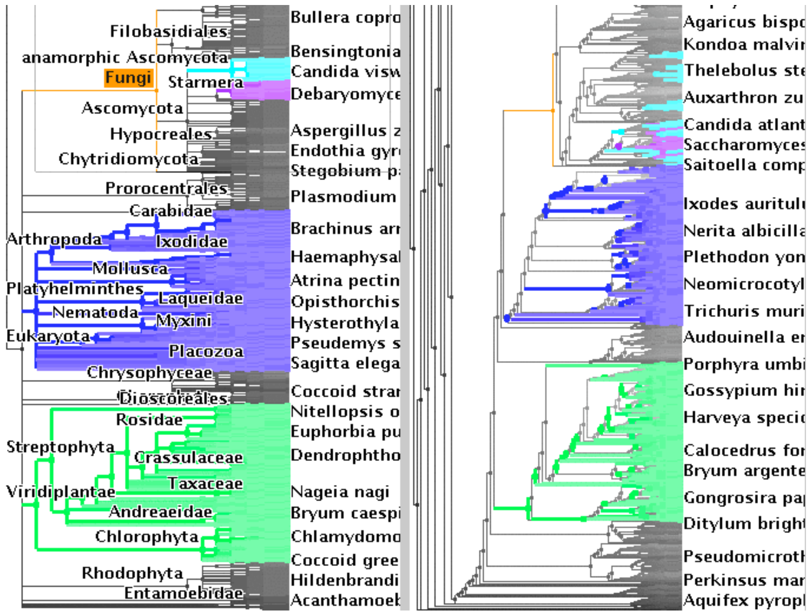
context



TreeJuxtaposer

- side by side comparison of evolutionary trees
- [video]
  - video/software downloadable from http://olduvai.sf.net/tj

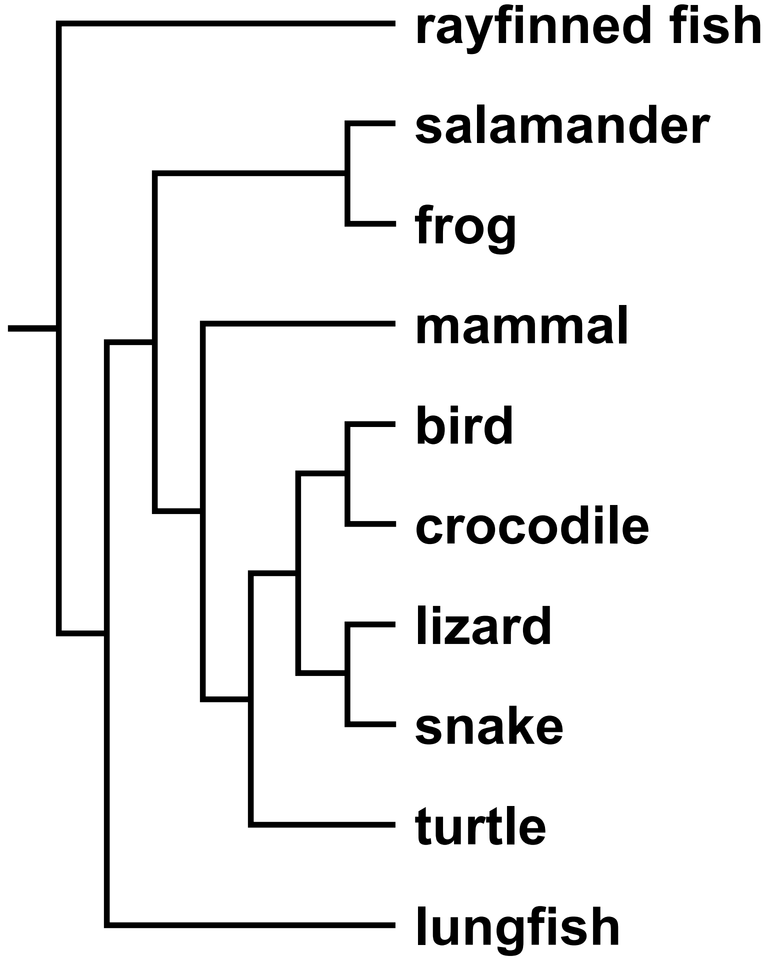


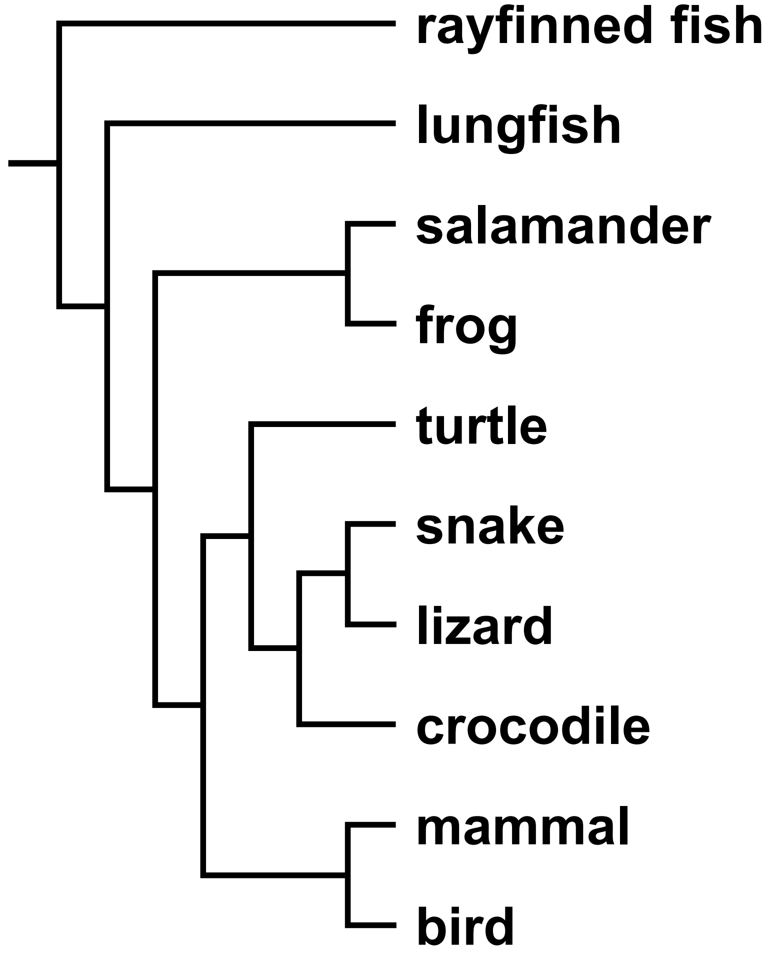


TJ Contributions

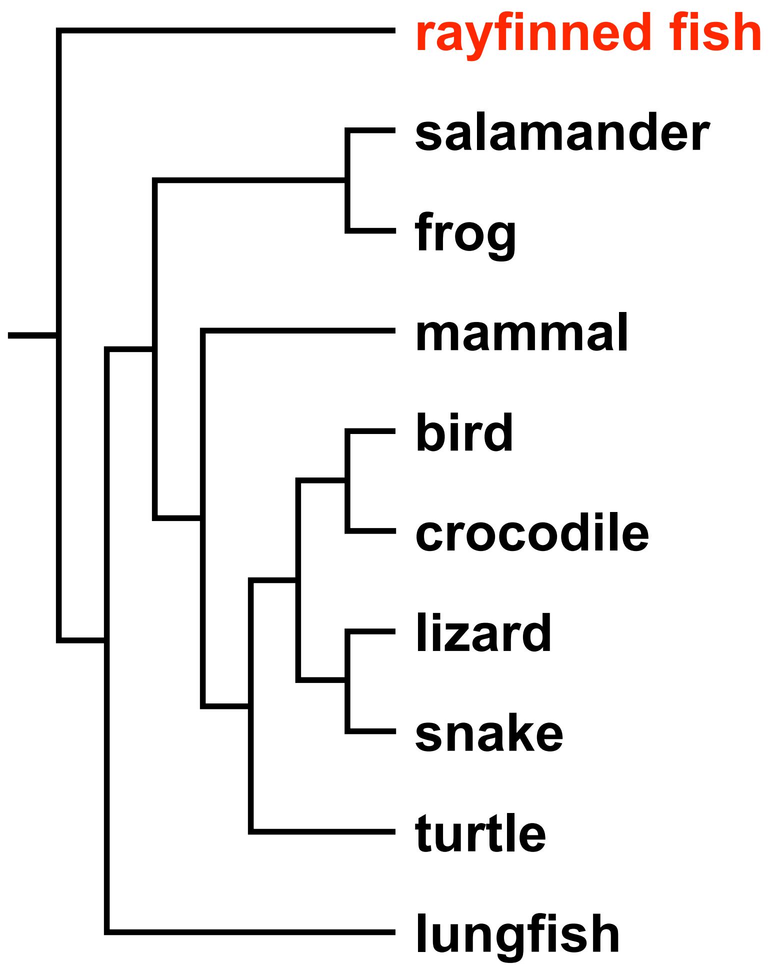
- first interactive tree comparison system
  - automatic structural difference computation
  - guaranteed visibility of marked areas
- scalable to large datasets
  - 250,000 to 500,000 total nodes
  - all preprocessing subquadratic
  - all realtime rendering sublinear
- scalable to large displays (4000 x 2000)
- introduced
  - guaranteed visibility, accordion drawing

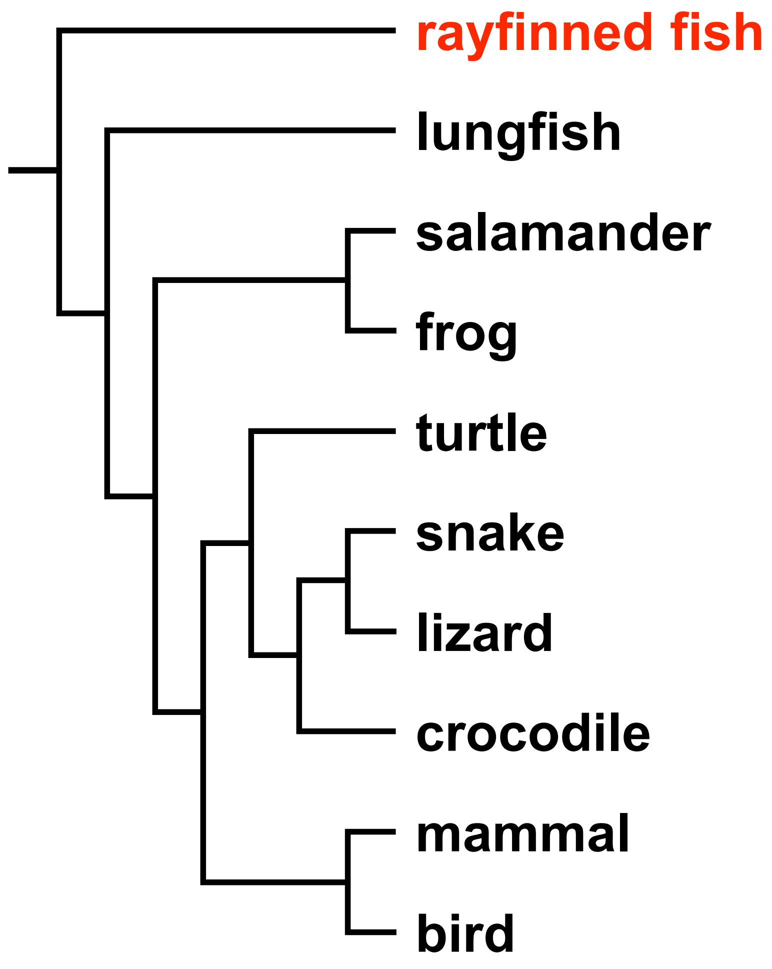
Structural Comparison





Matching Leaf Nodes





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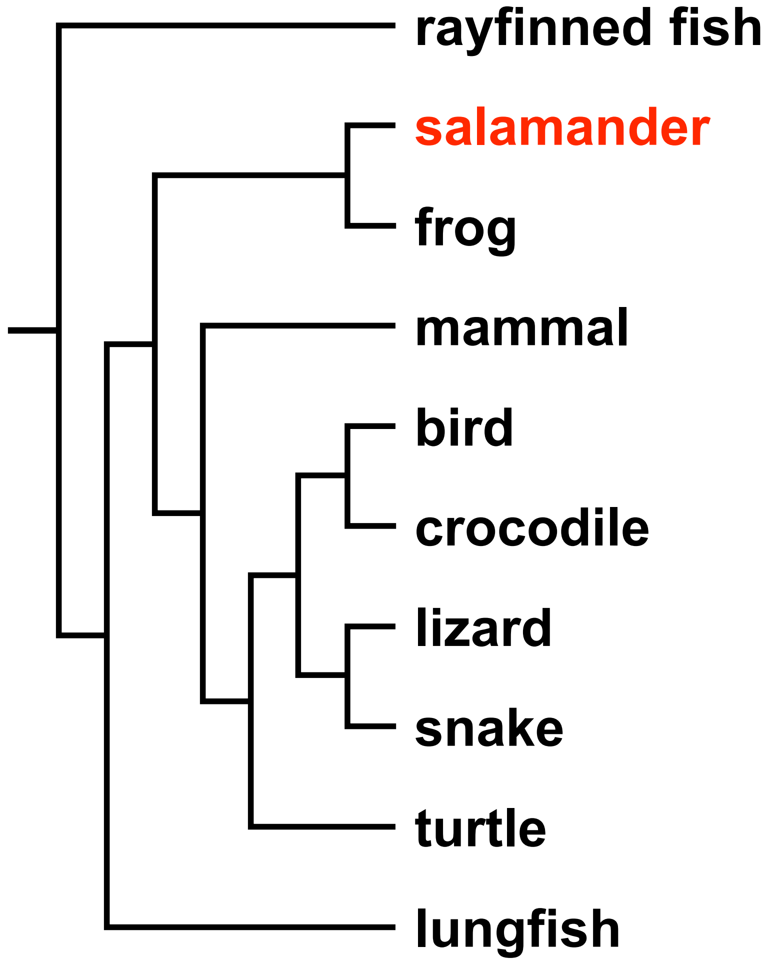

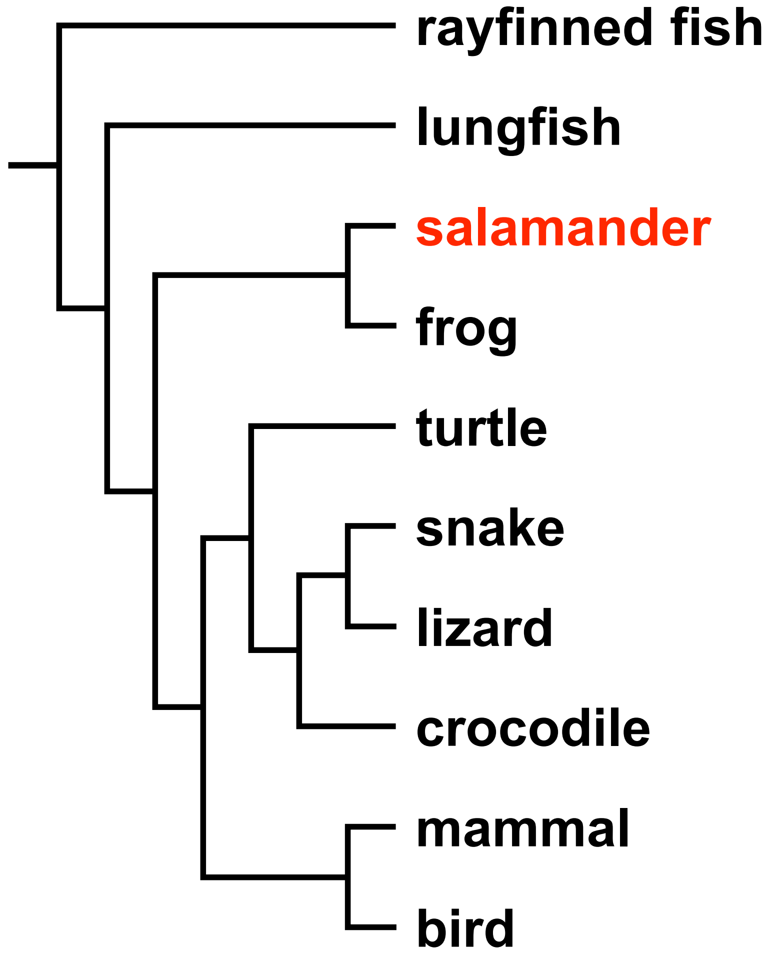

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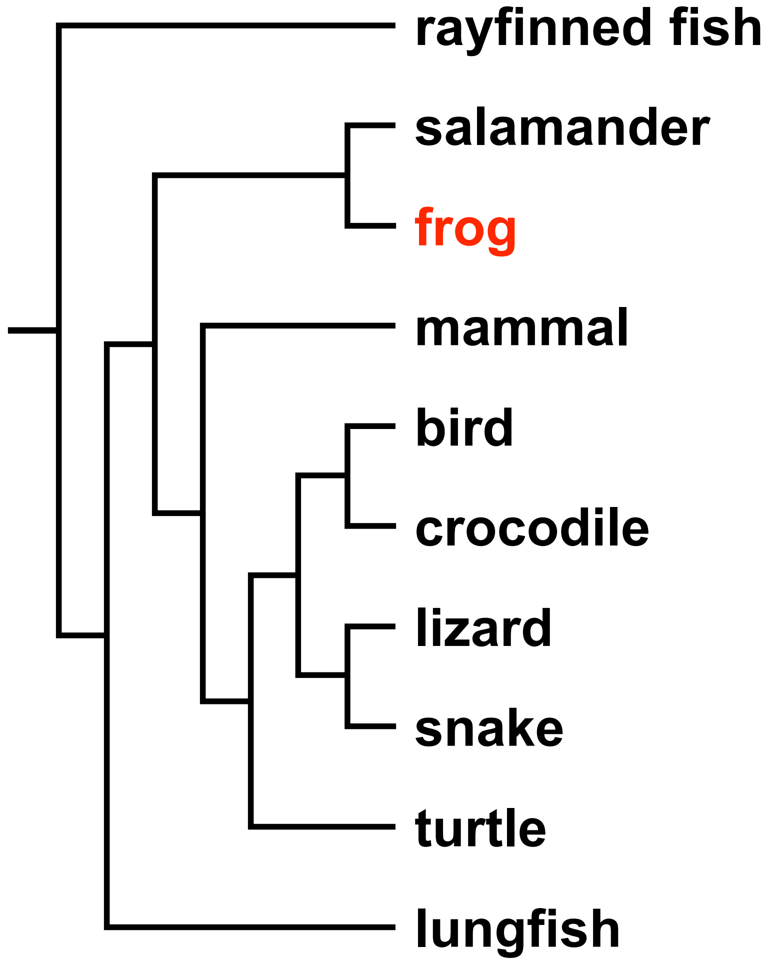
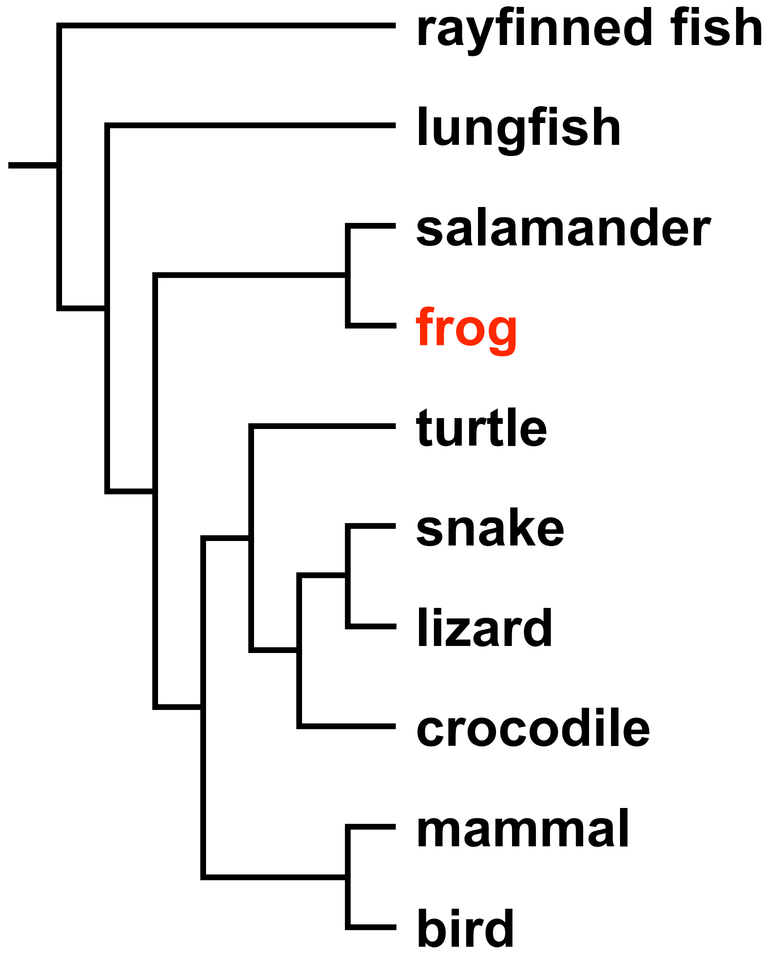
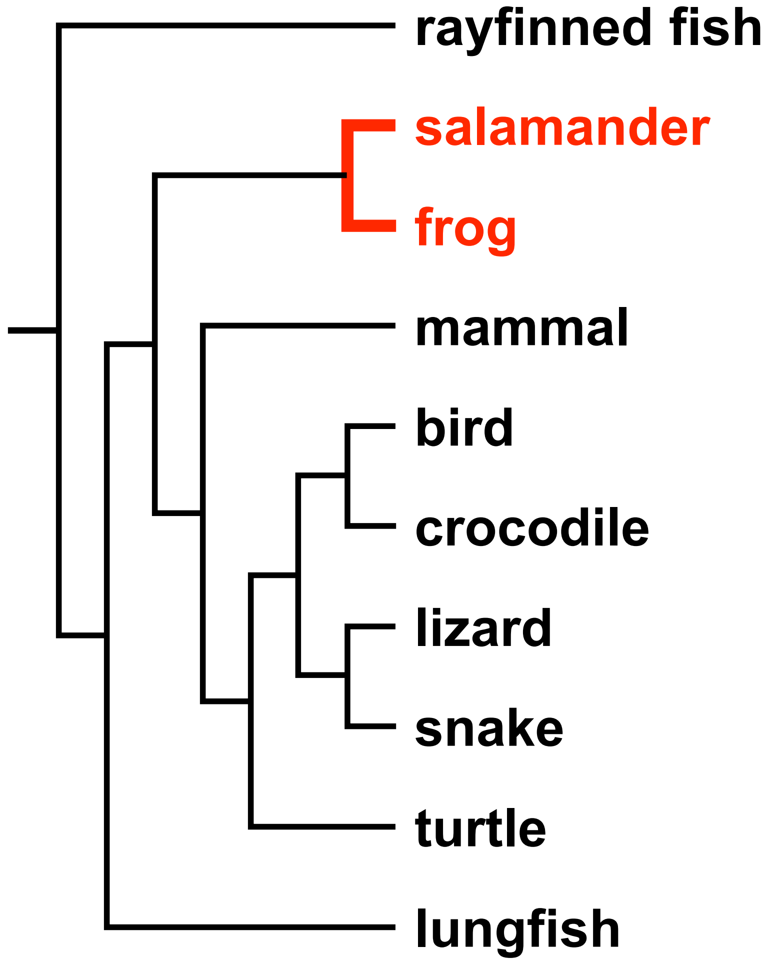
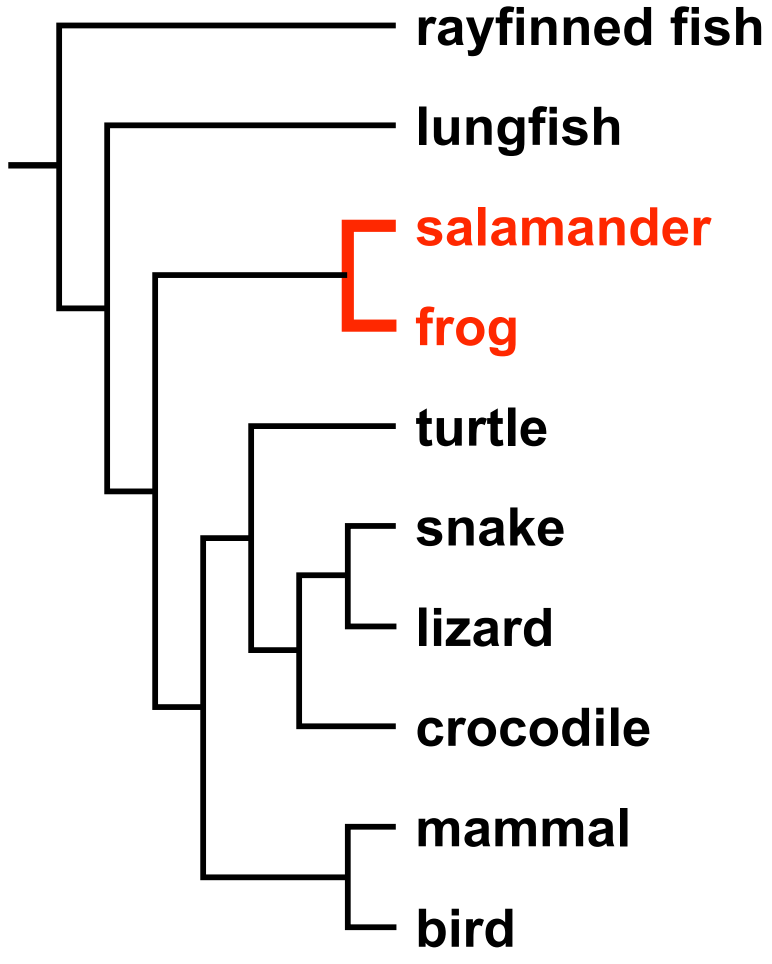


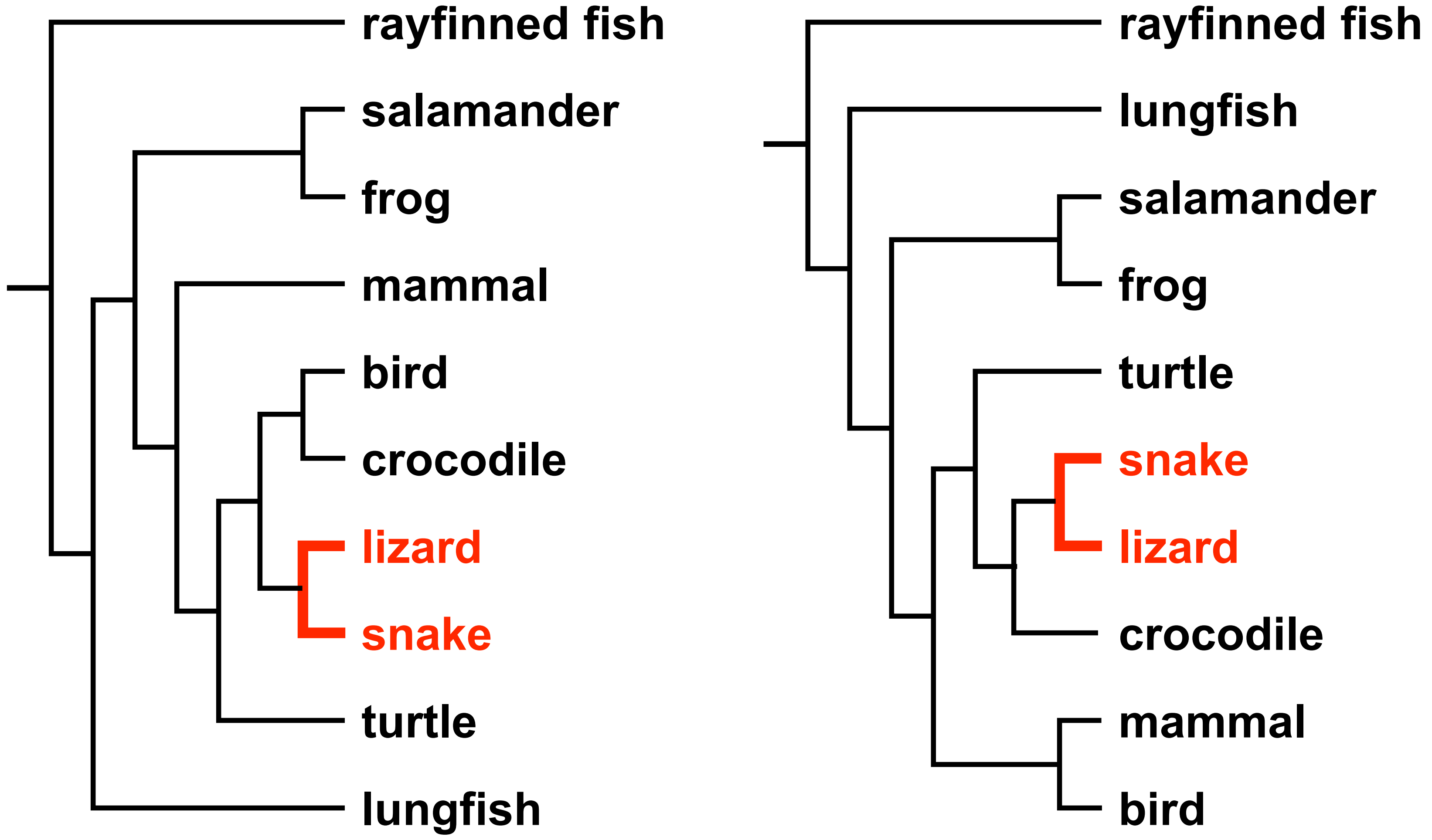


Matching Interior Nodes





Matching Interior Nodes



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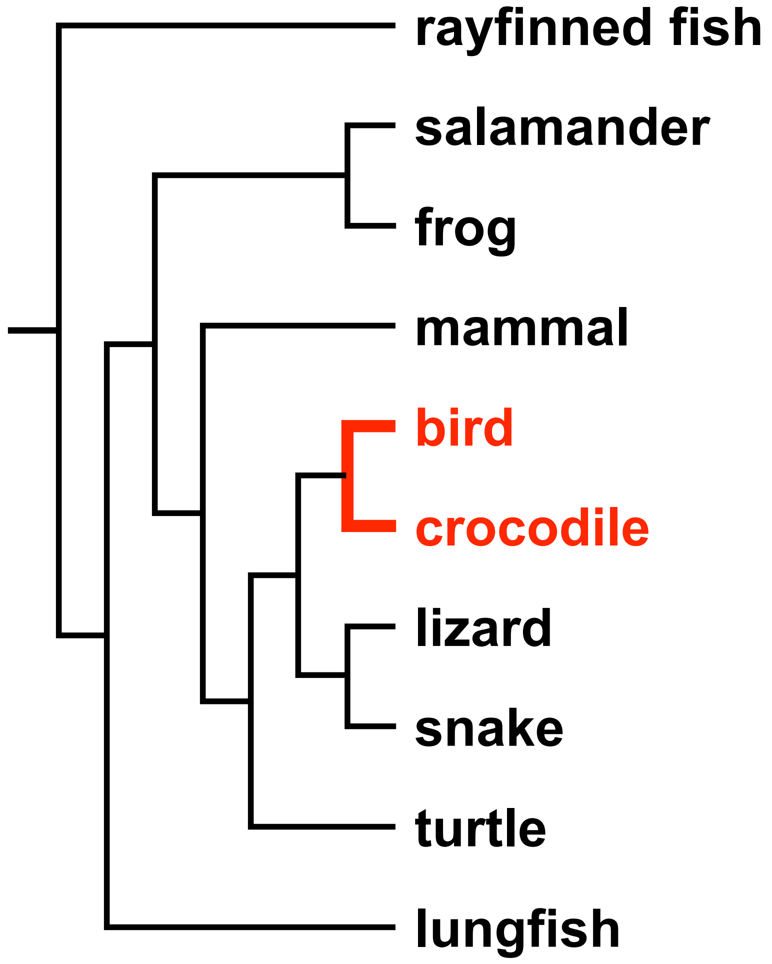

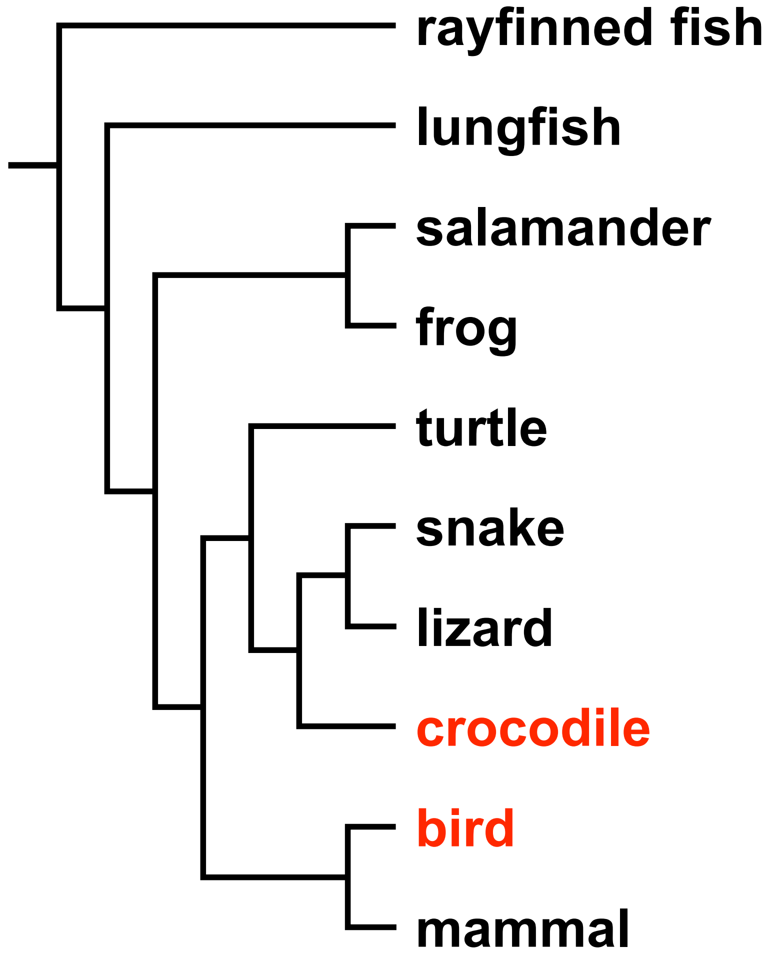

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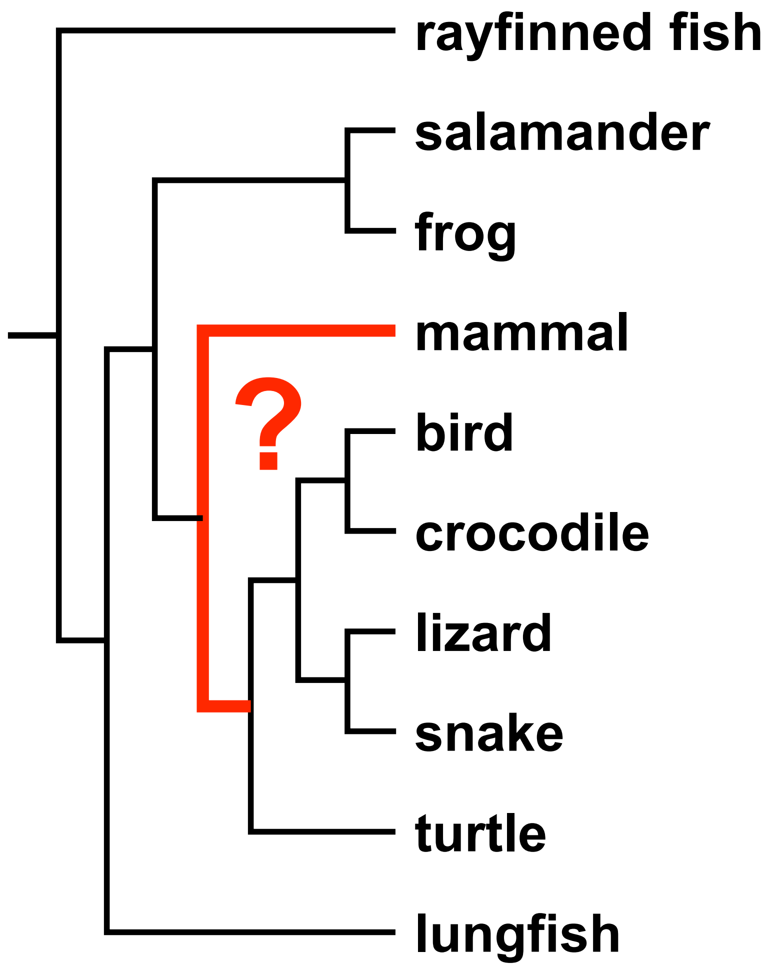
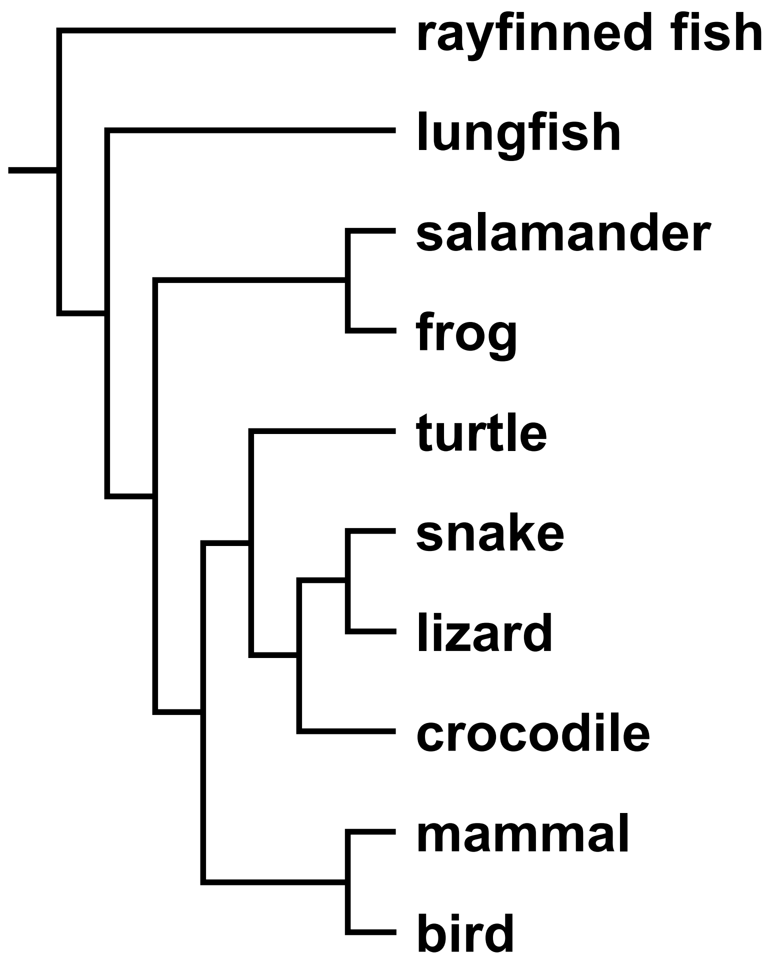
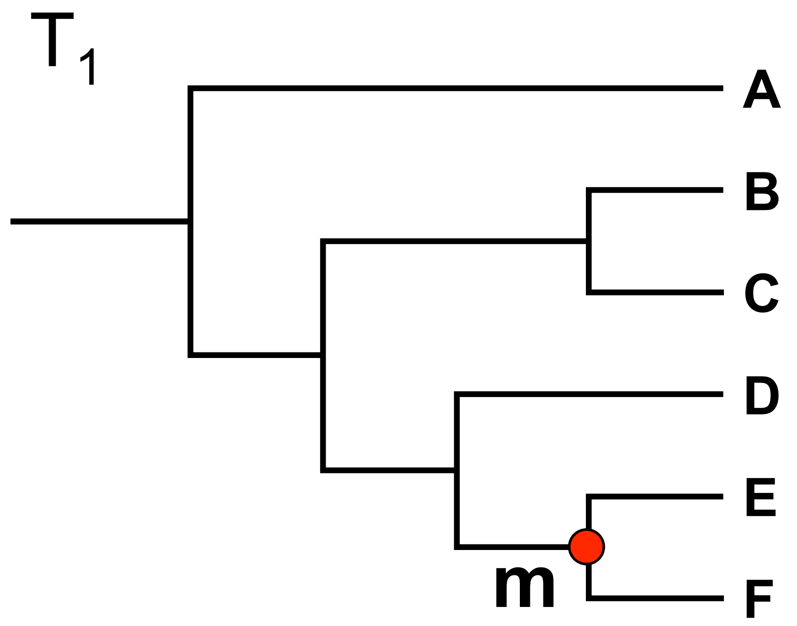


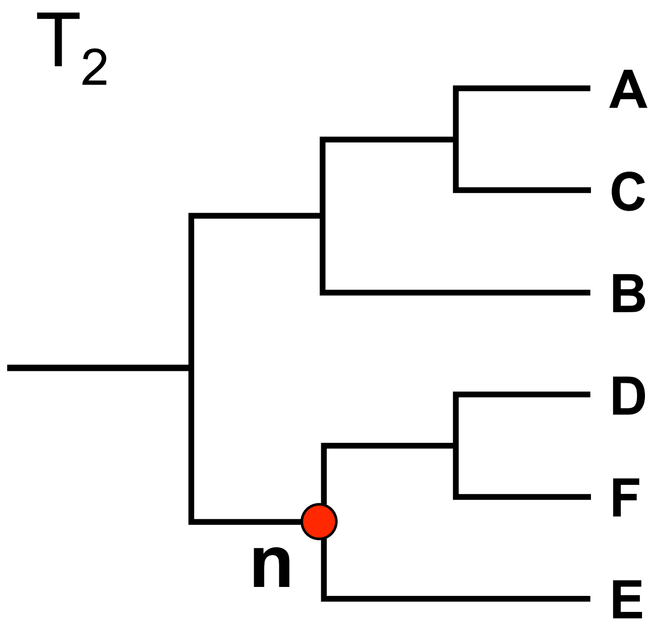


Previous Work

- tree comparison
  - RF distance [Robinson and Foulds 81]
  - perfect node matching [Day 85]
  - creation/deletion [Chi and Card 99]
  - leaves only [Graham and Kennedy 01]

Similarity Score: $S(\mathrm{m},\mathrm{n})$

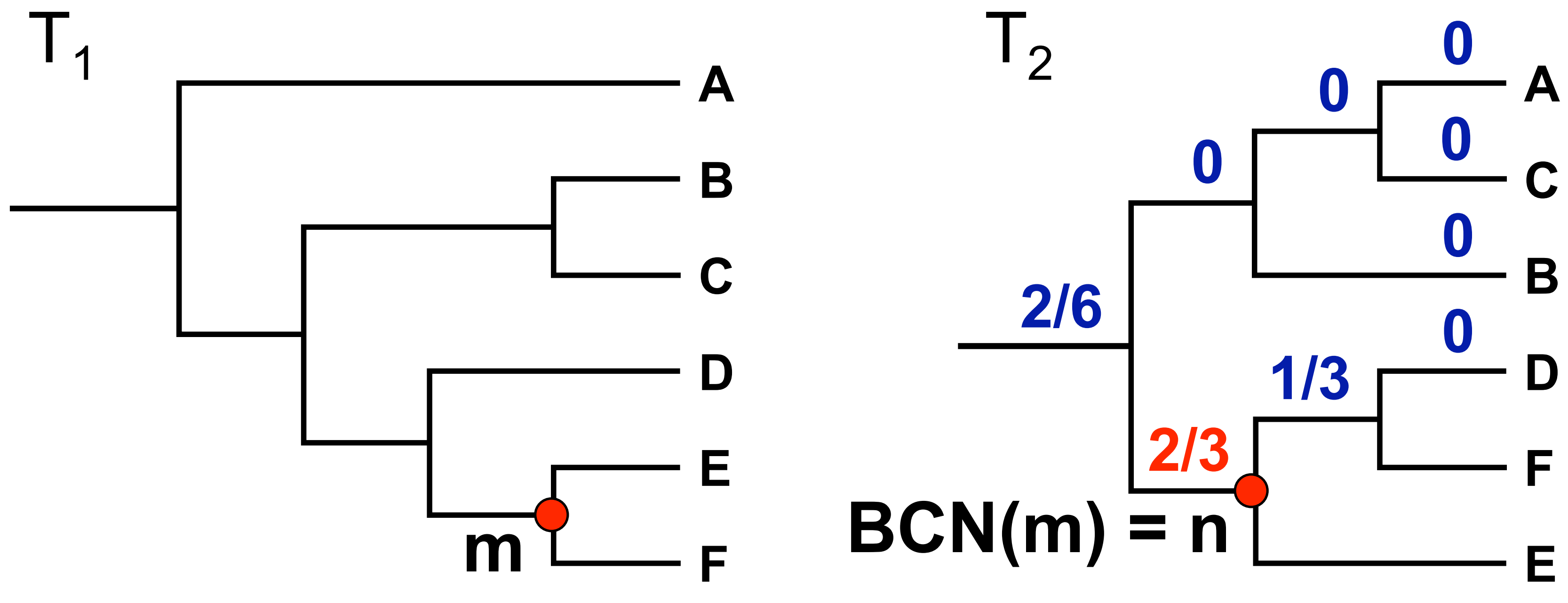




$L(\mathrm{m}) = \{\mathrm{E,F}\}$ $\qquad$ $L(\mathrm{n}) = \{\mathrm{D,E,F}\}$

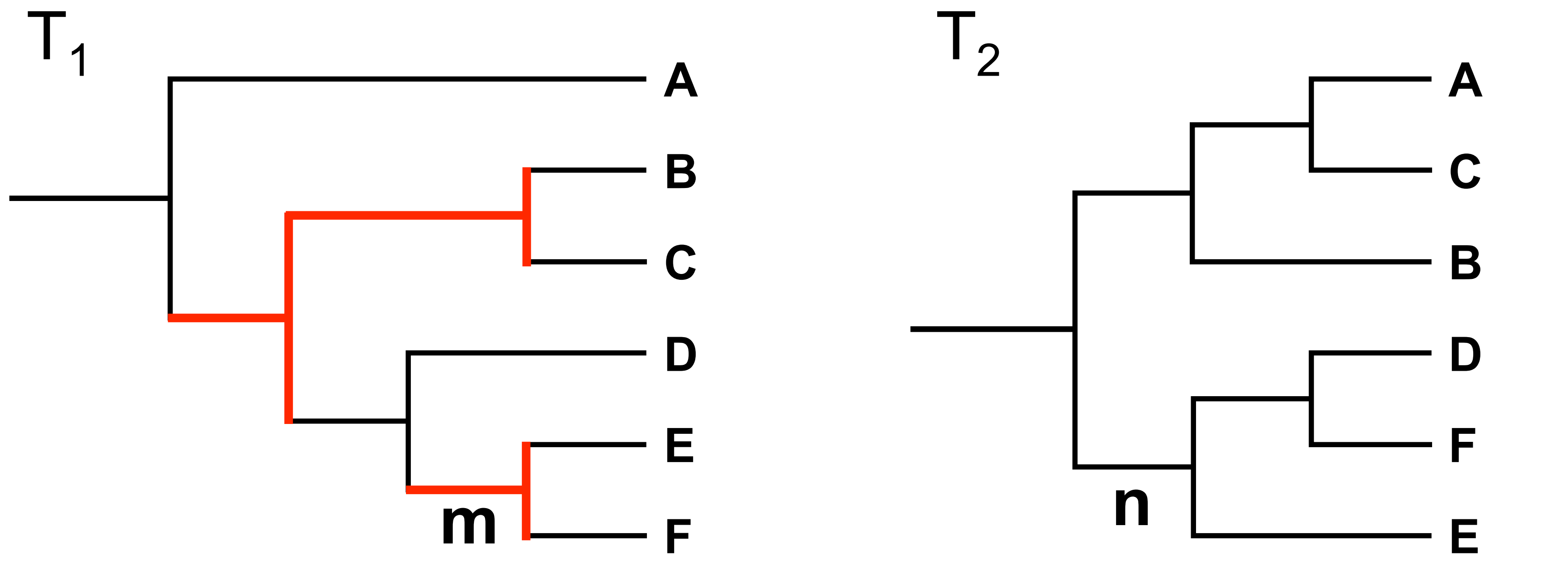
$$S(\mathrm{m},\mathrm{n}) = \frac{|L(\mathrm{m}) \cap L(\mathrm{n})|}{|L(\mathrm{m}) \cup L(\mathrm{n})|} = \frac{|\{\mathrm{E,F}\}|}{|\{\mathrm{D,E,F}\}|} = \frac{2}{3}$$

Best Corresponding Node



- $\text{BCN}(m) = \text{argmax}_{v \in T_2}(S(m, v))$
  - computable in $O(n \log^2 n)$
  - linked highlighting

Marking Structural Differences



- Nodes for which $S(v,\text{BCN}(v)) \neq 1$
  - Matches intuition

Outline

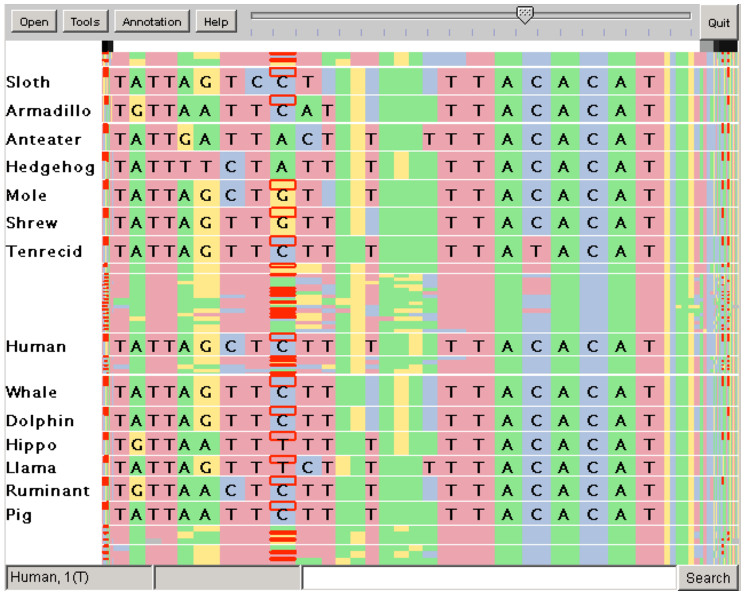
- Accordion Drawing
  - information visualization technique
- TreeJuxtaposer
  - tree comparison
- SequenceJuxtaposer
  - sequence comparison
- PRISAD
  - generic accordion drawing framework

Genomic Sequences

- multiple aligned sequences of DNA
- now commonly browsed with web apps
  - zoom and pan with abrupt jumps
  - previous work
    - Ensembl [Hubbard 02], UCSC Genome Browser [Kent 02], NCBI [Wheeler 02]
- investigate benefits of accordion drawing
  - showing focus areas in context
  - smooth transitions between states
  - guaranteed visibility for globally visible landmarks

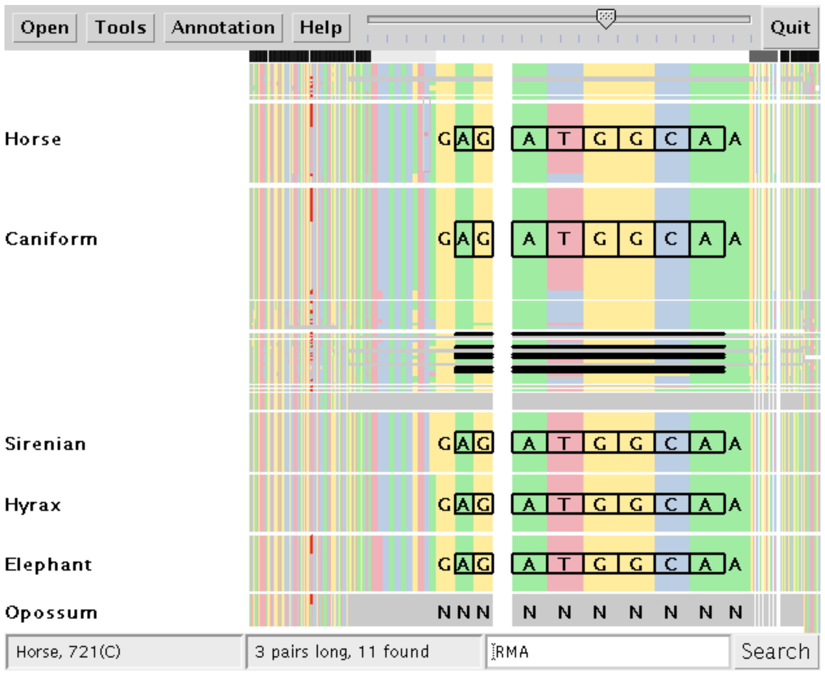
SequenceJuxtaposer

- comparing multiple aligned gene sequences
- provides searching, difference calculation
- [video]
  - video/software downloadable from http://olduvai.sf.net/tj



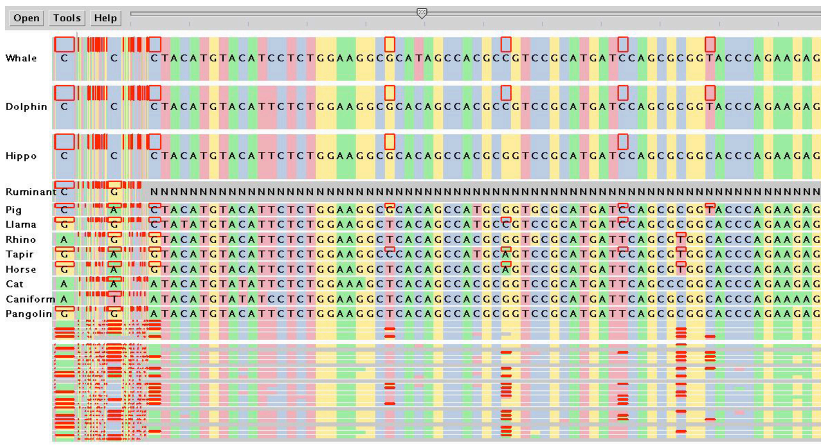
Searching

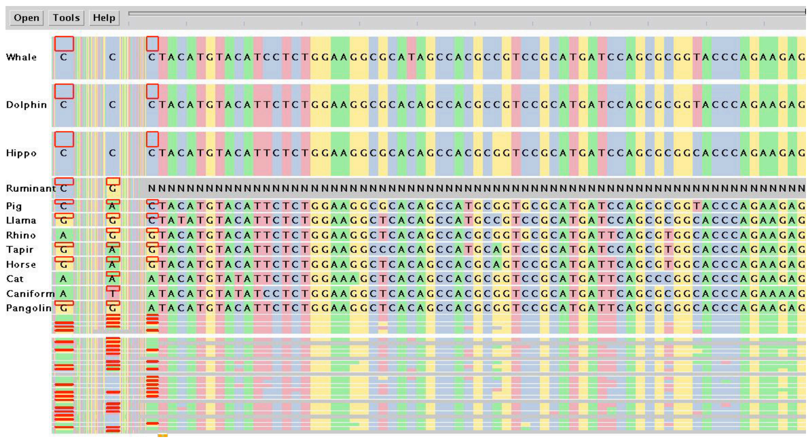
- search for motifs
  - protein/codon search
  - regular expressions supported
- results marked with guaranteed visibility



Differences

- explore differences between aligned pairs
  - slider controls difference threshold in realtime
- results marked with guaranteed visibility





SJ Contributions

- fluid tree comparison system
  - showing multiple focus areas in context
  - guaranteed visibility of marked areas
    - thresholded differences, search results
- scalable to large datasets
  - 2M nucleotides
  - all realtime rendering sublinear

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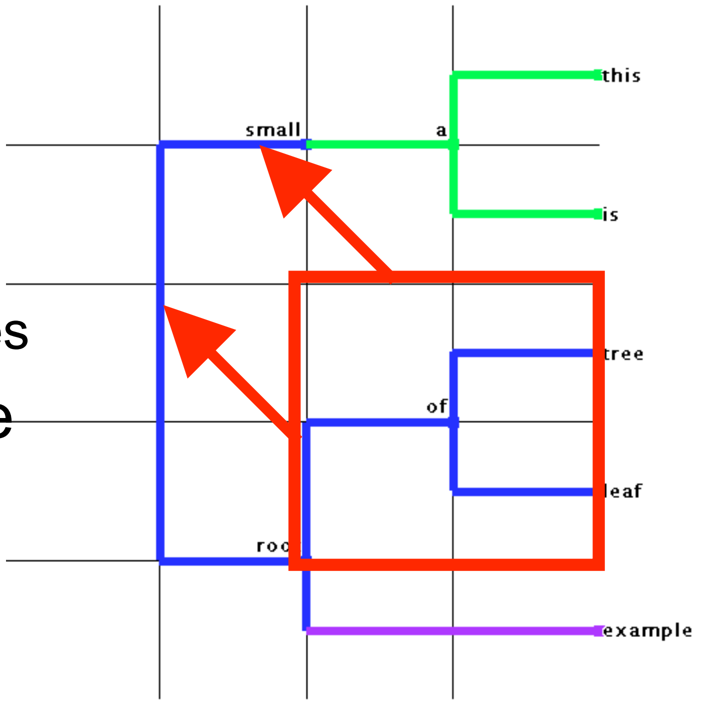
Goals of PRISAD

- generic AD infrastructure
  - tree and sequence applications
    - PRITree is TreeJuxtaposer using PRISAD
    - PRISeq is SequenceJuxtaposer using PRISAD
- efficiency
  - faster rendering: minimize overdrawing
  - smaller memory footprint
- correctness
  - rendering with no gaps: eliminate overculling

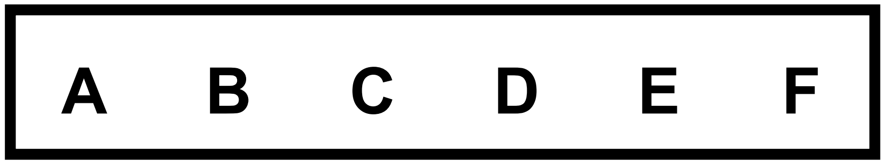
PRISAD Navigation

- generic navigation infrastructure
  - application independent
  - uses deformable grid
  - split lines
    - Grid lines define object boundaries
  - horizontal and vertical separate
    - Independently movable

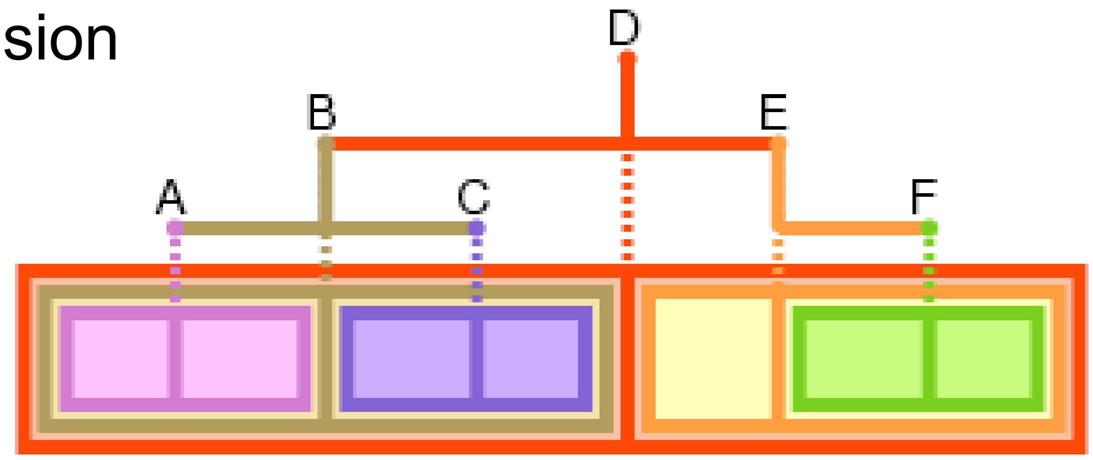


Split line hierarchy

- data structure supports navigation, picking, drawing
- two interpretations
  - linear ordering

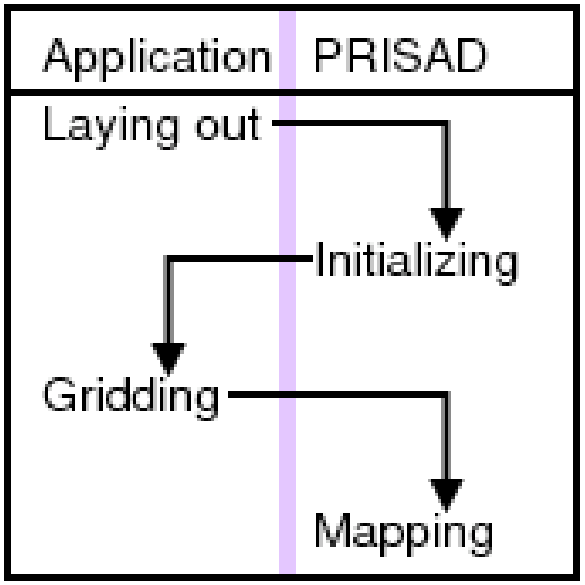


  - hierarchical subdivision

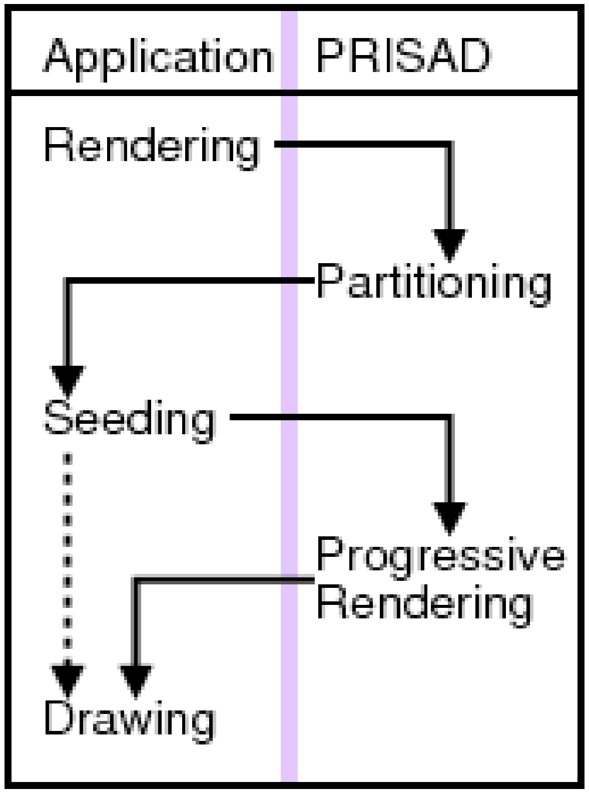


PRISAD Architecture

world-space discretization
- preprocessing
  - initializing data structures
  - placing geometry

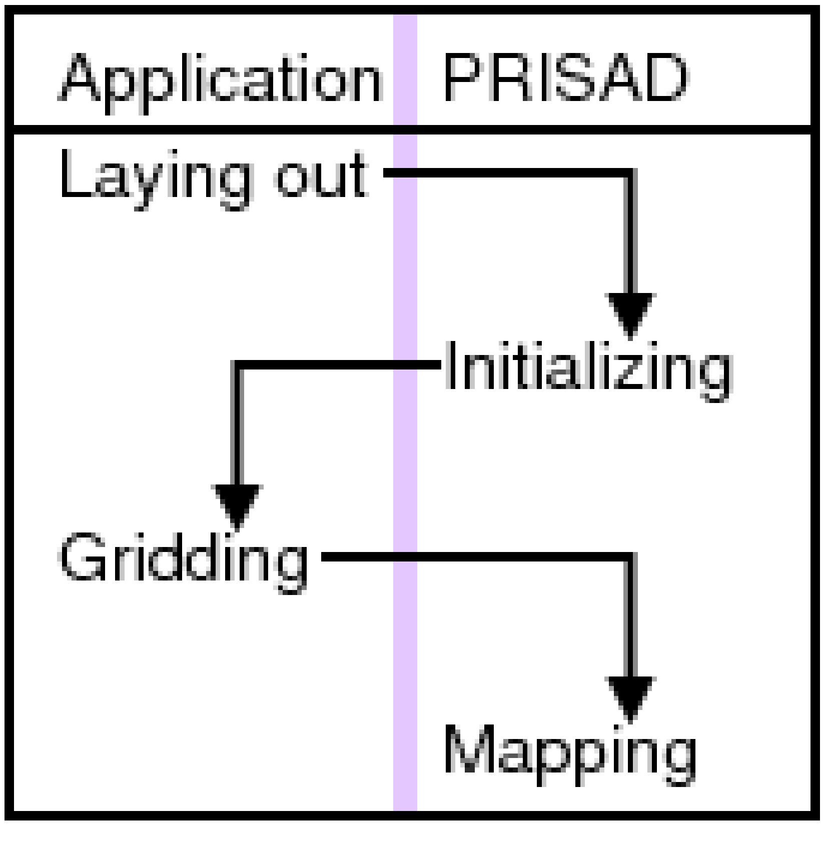


screen-space rendering
- frame updating
  - analyzing navigation state
  - drawing geometry



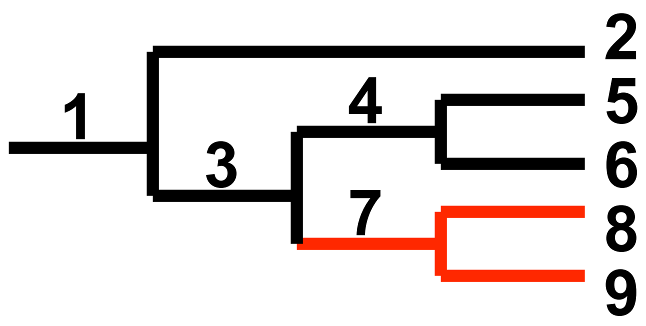
World-space Discretization

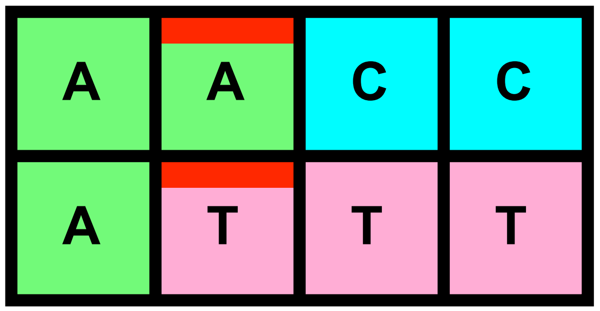
interplay between infrastructure and application



Laying Out & Initializing

- application-specific layout of dataset
  – non-overlapping objects
- initialize PRISAD split line hierarchies
  – objects aligned by split lines





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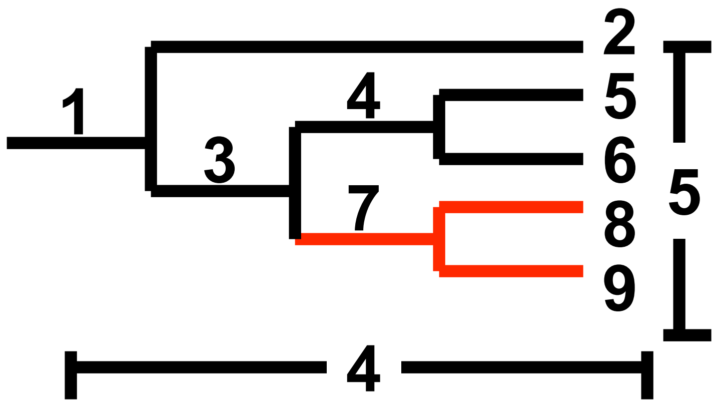
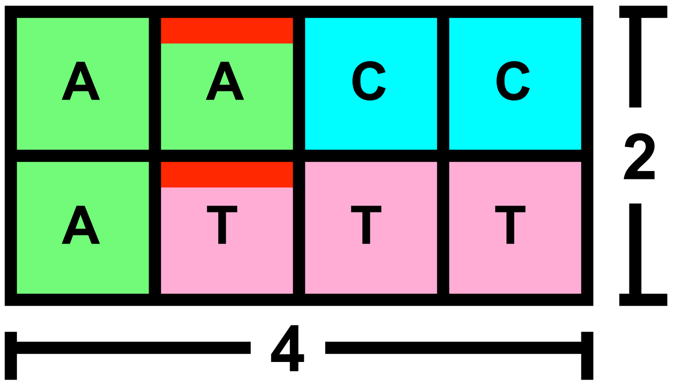
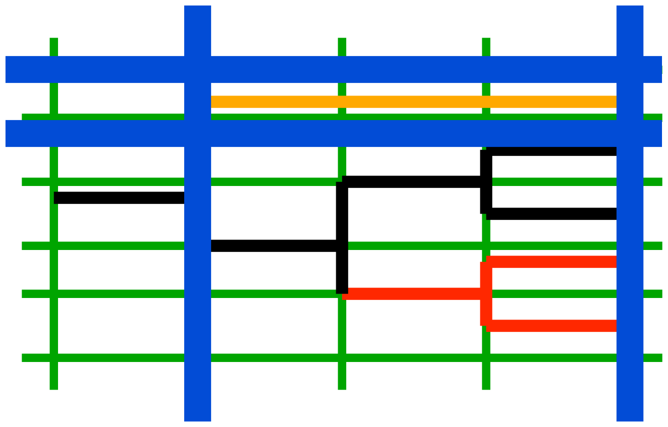
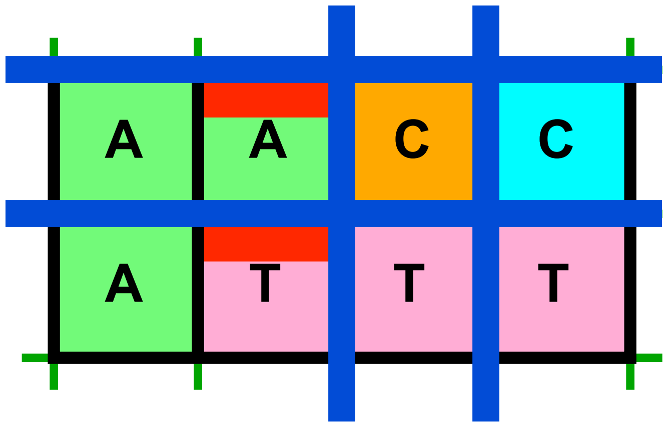




Gridding

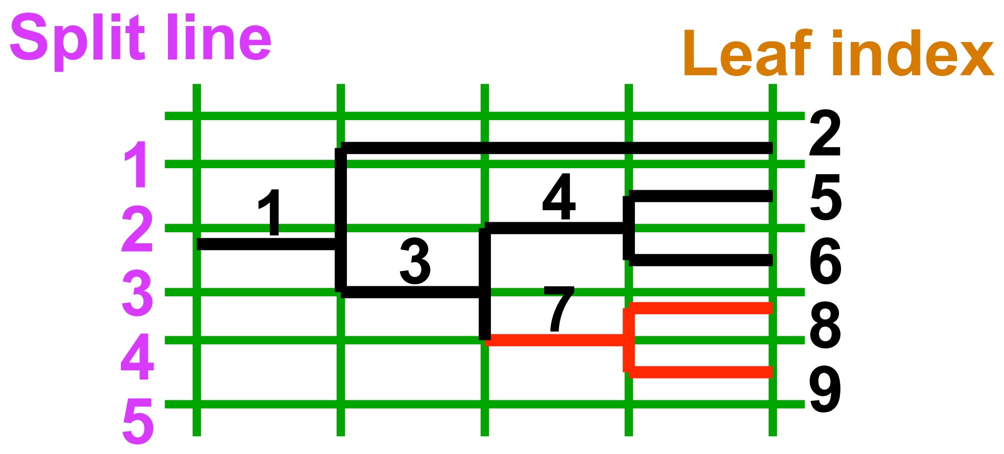
- each geometric object assigned its four encompassing split line boundaries





Mapping

- PRITree mapping initializes leaf references
  - bidirectional O(1) reference between leaves and split lines

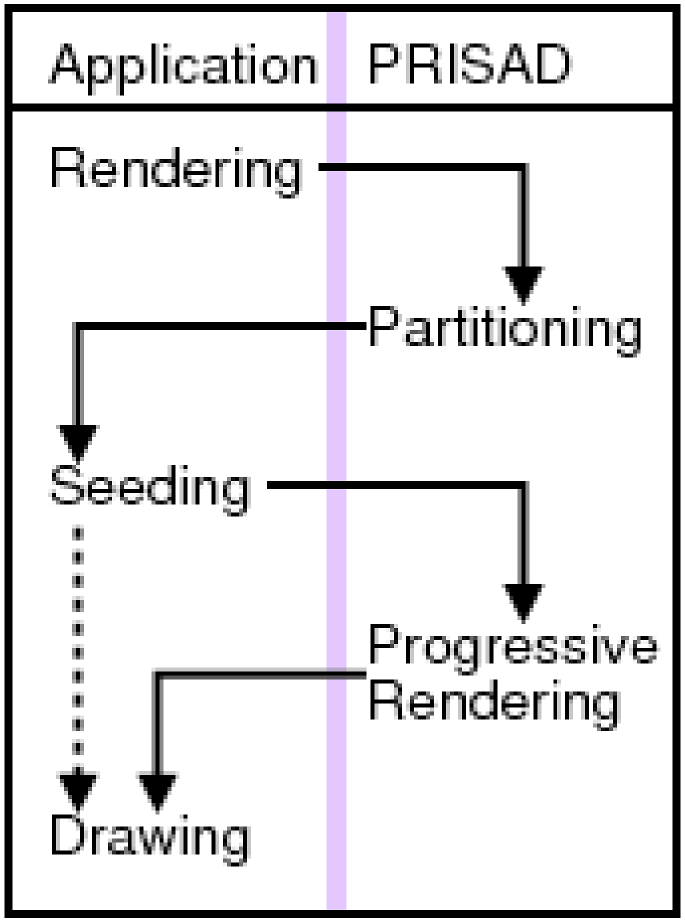


Map

1	2
2	5
3	6
4	8
5	9

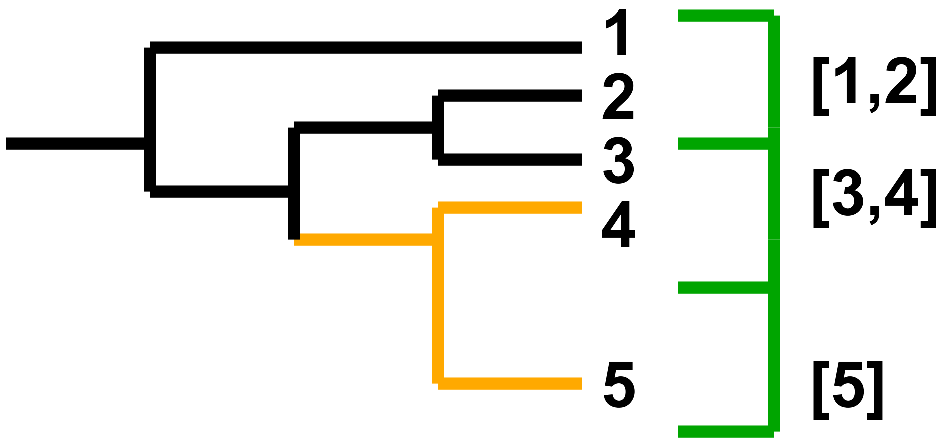
Screen-space Rendering

control flow to draw each frame



Partitioning

- partition object set into bite-sized ranges
  - using current split line screen-space positions
    - required for every frame
  - subdivision stops if region smaller than 1 pixel
    - or if range contains only 1 object

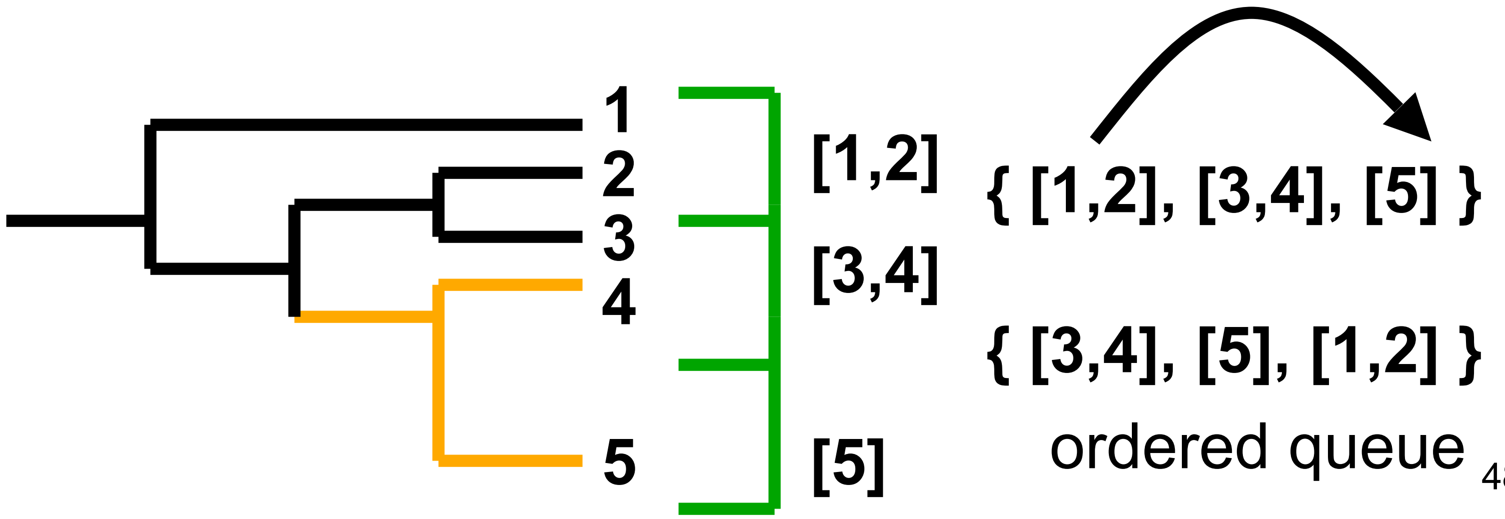


{ [1,2], [3,4], [5] }

Queue of ranges

Seeding

- reordering range queue result from partition
  - marked regions get priority in queue
    - drawn first to provide landmarks

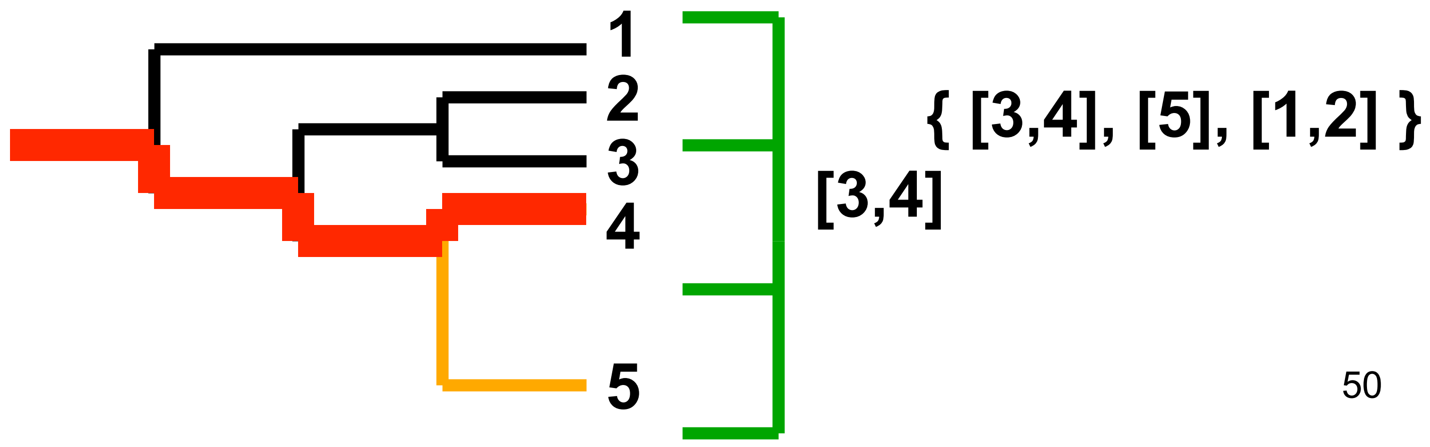


Drawing Single Range

- each enqueued object range drawn according to application geometry
  - selection for trees
  - aggregation for sequences

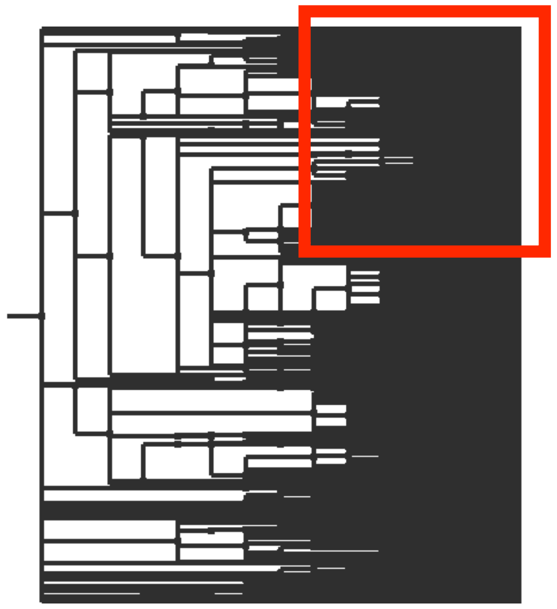
PRITree Range Drawing

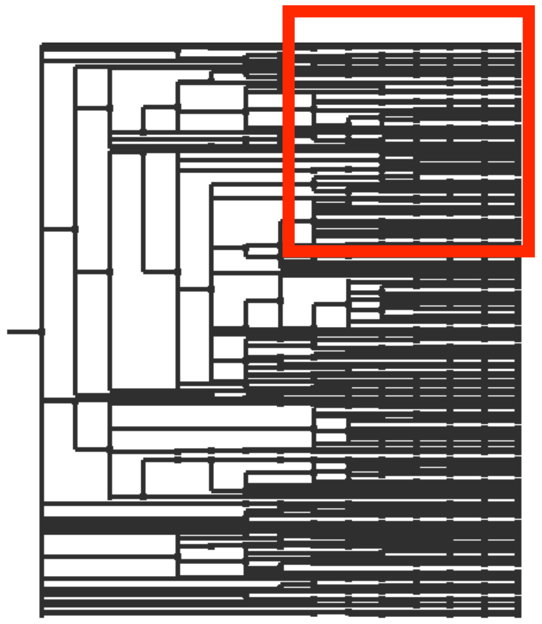
- select suitable leaf in each range
- draw path from leaf to the root
  - ascent-based tree drawing
  - efficiency: minimize overdrawing
    - only draw one path per range



Rendering Dense Regions

- correctness: eliminate overculling
  - bad leaf choices would result in misleading gaps
- efficiency: maximize partition size to reduce rendering
  - too much reduction would result in gaps


Intended rendering


Partition size too big

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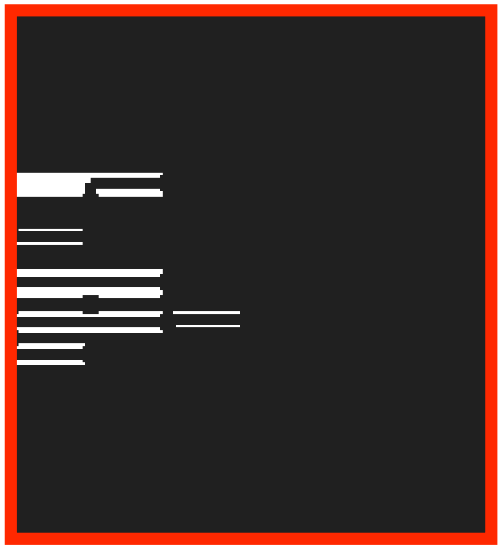
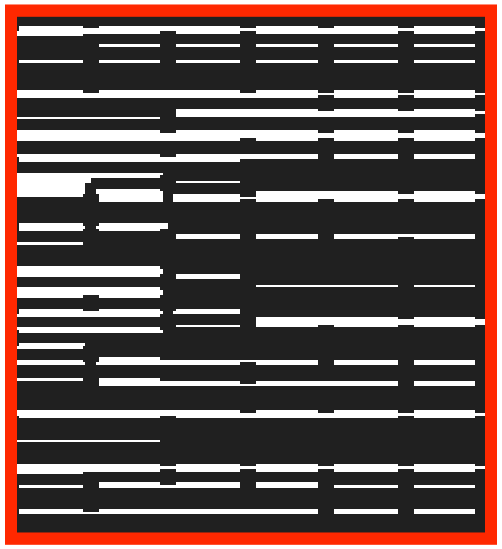
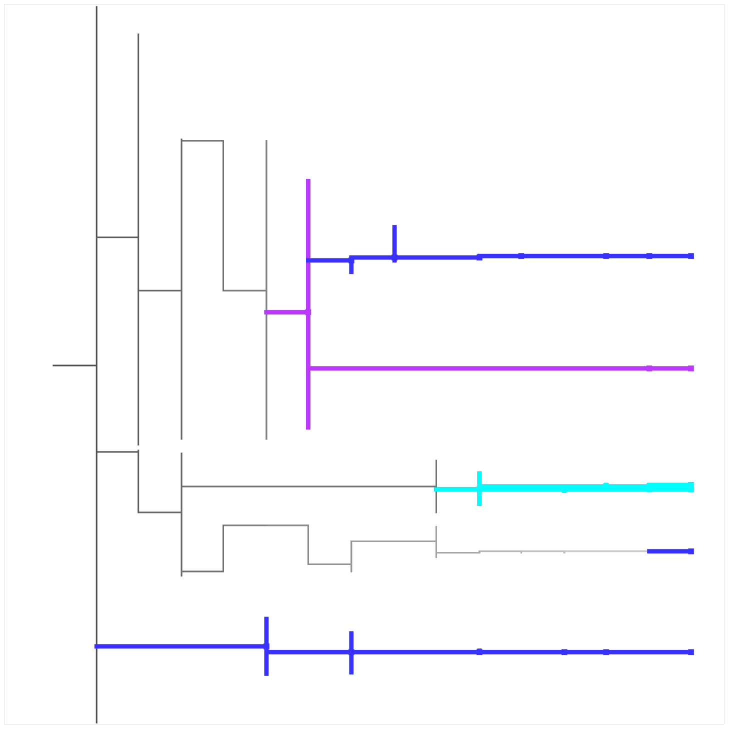

Intended rendering


Partition size too big

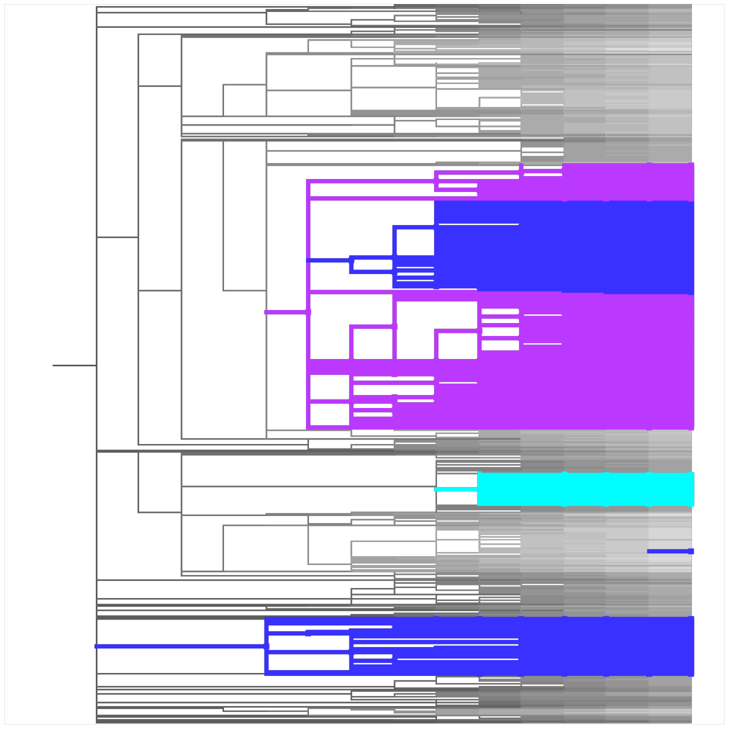
PRITree Skeleton

- guaranteed visibility of marked subtrees during progressive rendering

first frame: one path per marked group

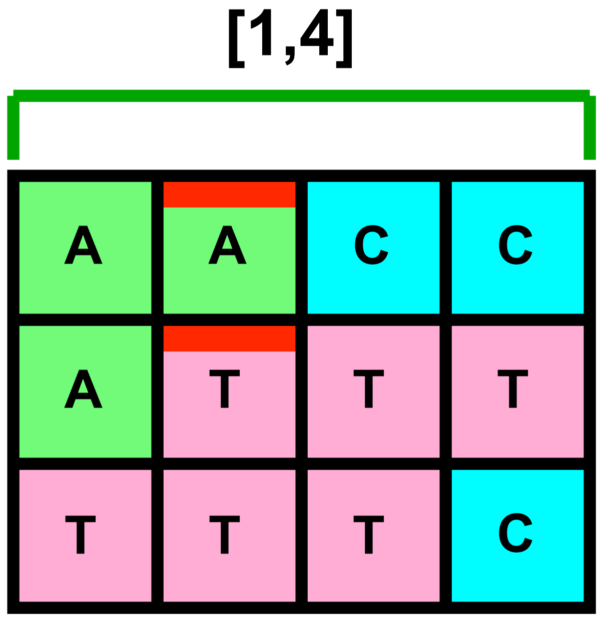


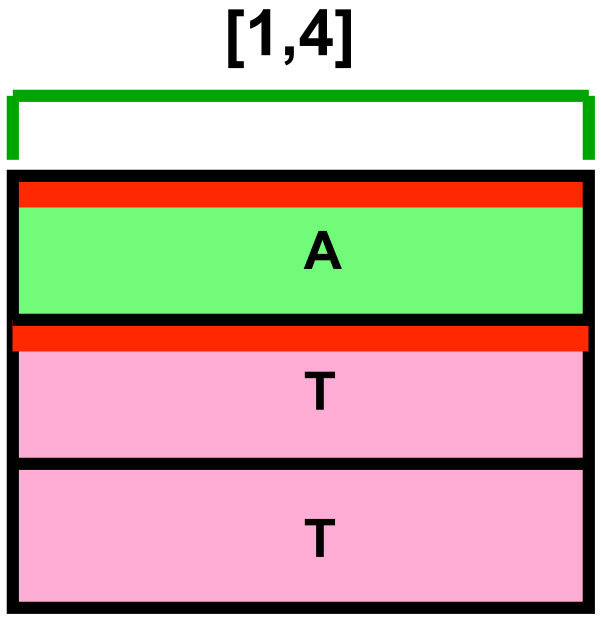
full scene: entire marked subtrees



PRISeq Range Drawing: Aggregation

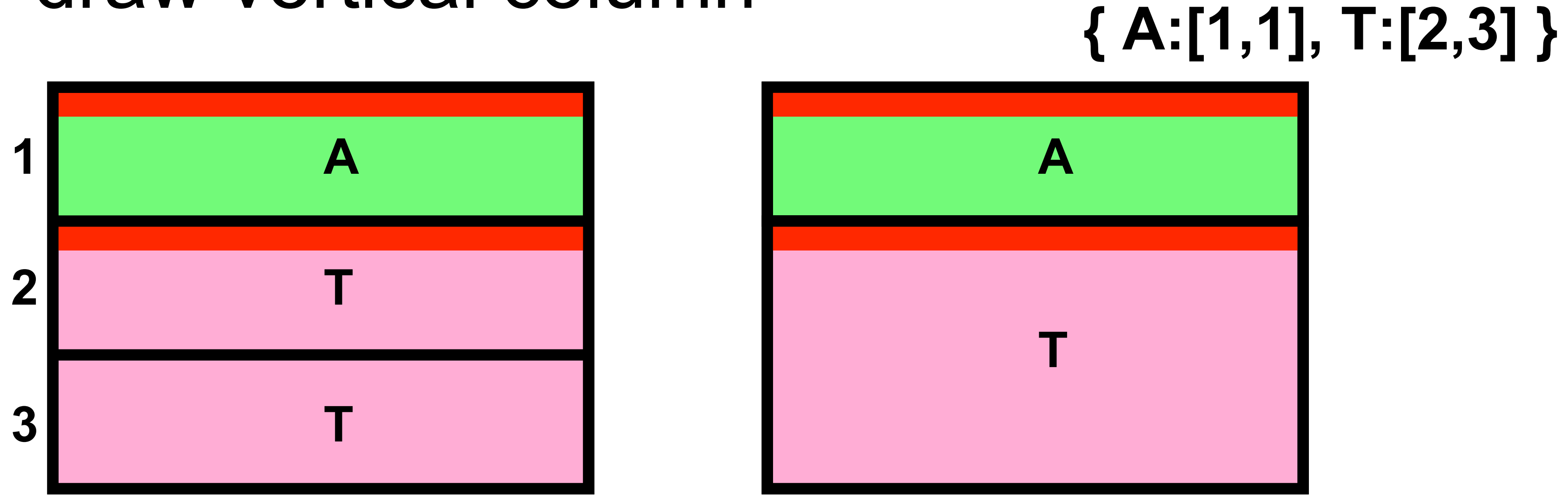
- aggregate range to select box color for each sequence
  - random select to break ties





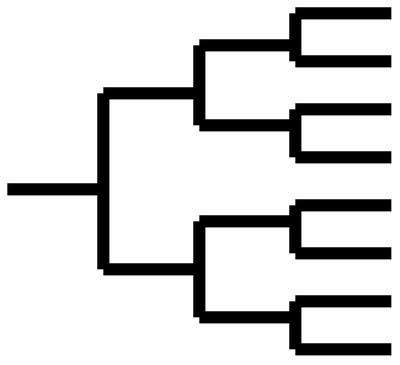
PRISeq Range Drawing

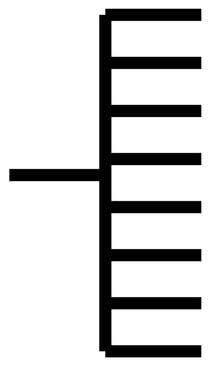
- collect identical nucleotides in column
  - form single box to represent identical objects
    - attach to split line hierarchy cache
    - lazy evaluation
- draw vertical column



PRISAD Performance

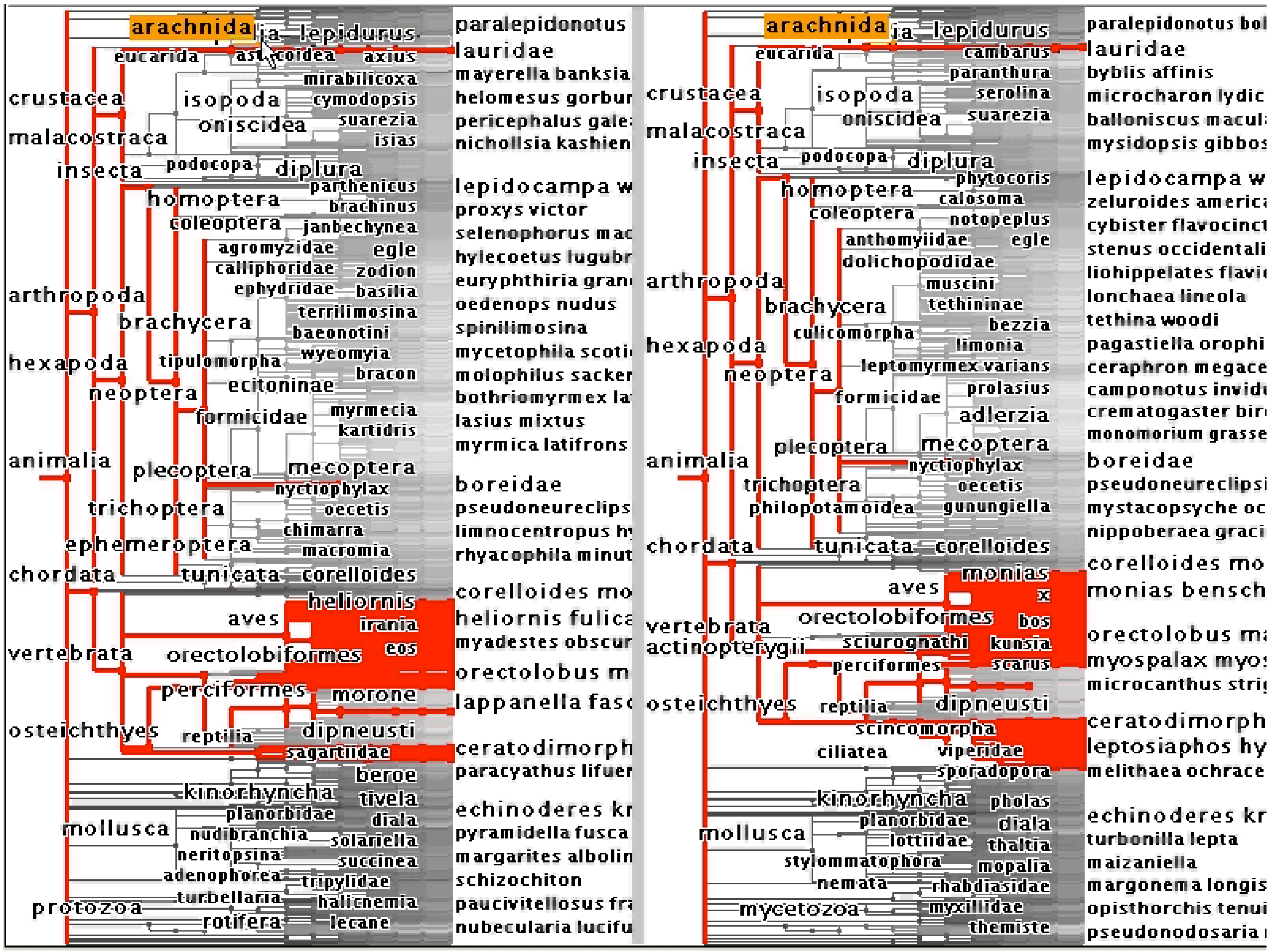
- PRITree vs. TreeJuxtaposer (TJ)
- synthetic and real datasets
  - complete binary trees
    - lowest branching factor
    - regular structure
  - star trees
    - highest possible branching factor





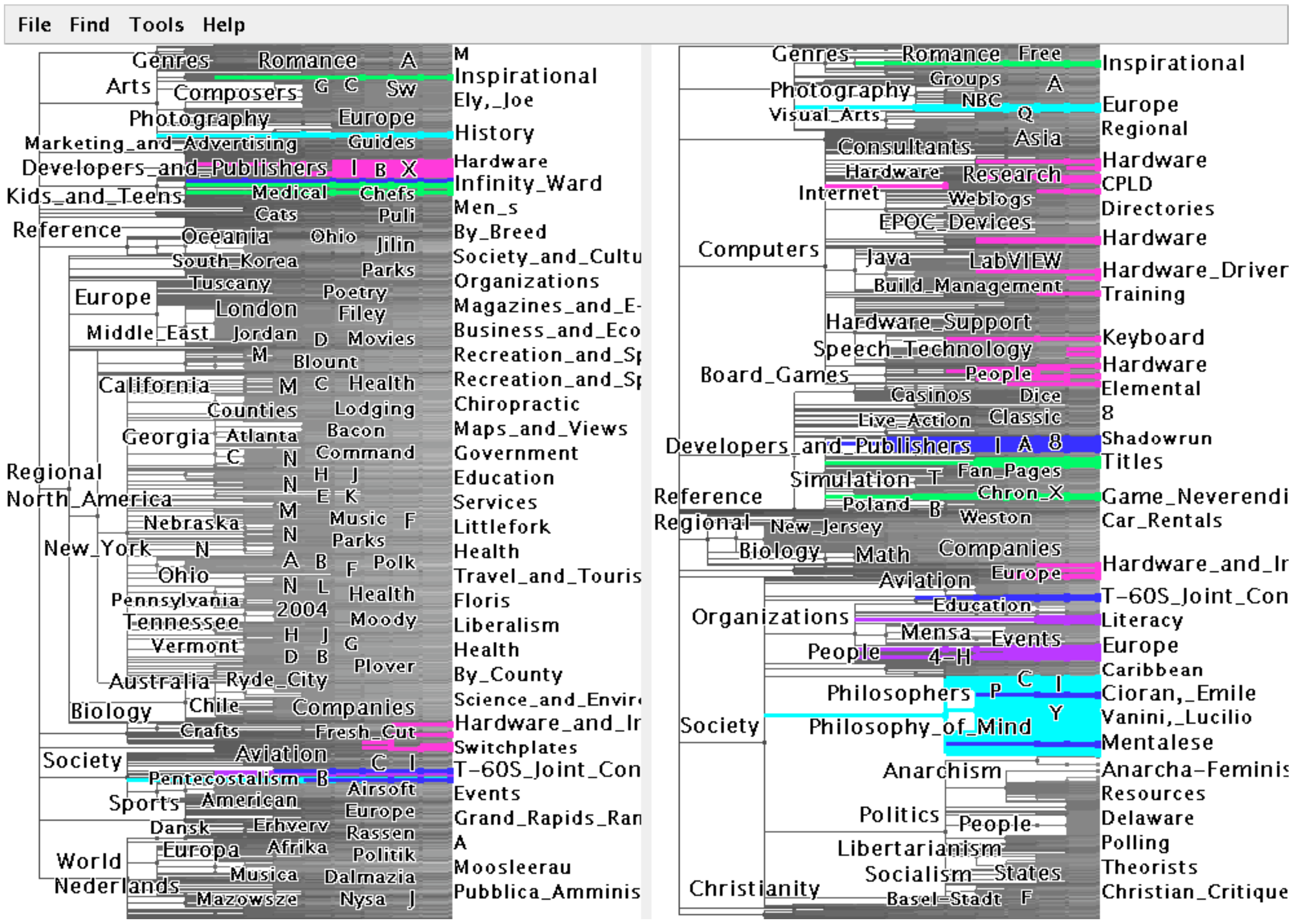
InfoVis Contest Benchmarks

- two 190K node trees
- directly compare TJ and PT



OpenDirectory benchmarks

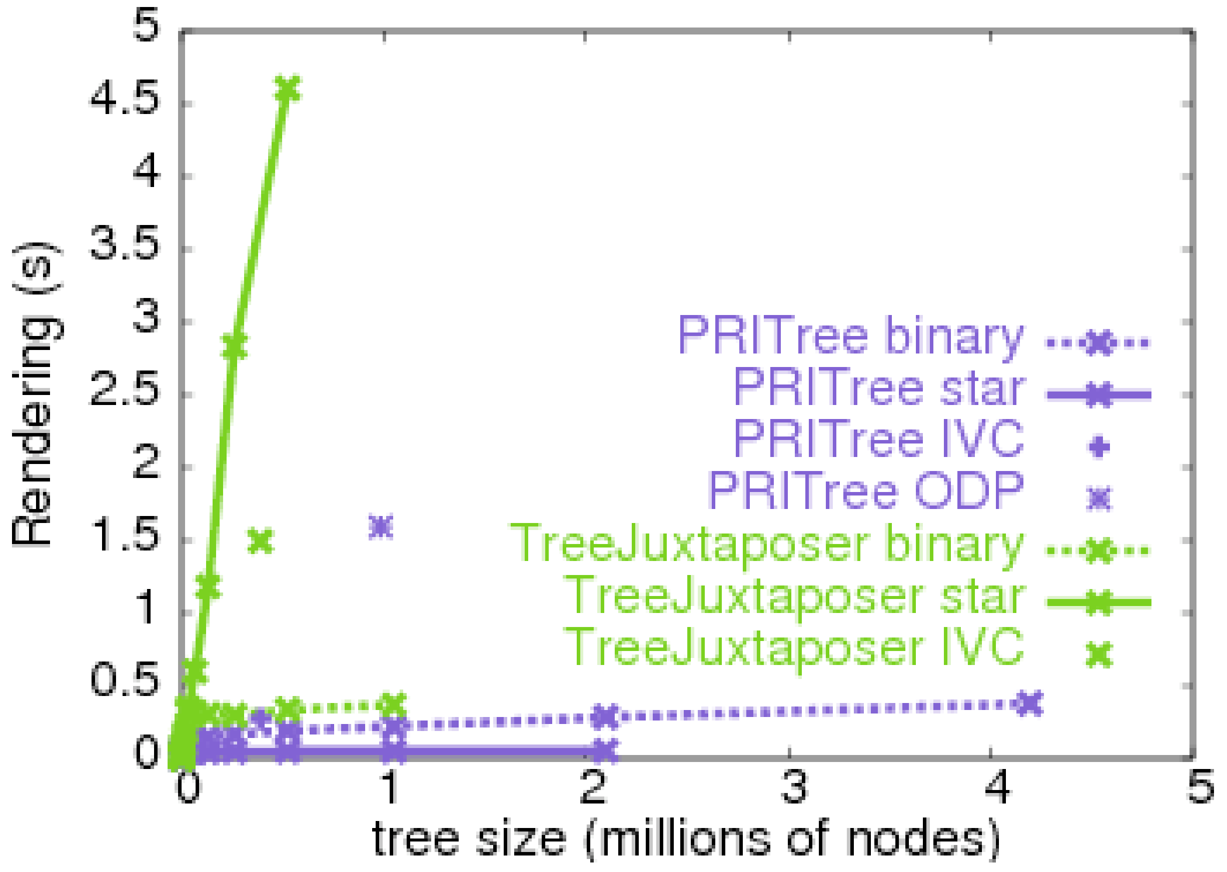
- two 480K node trees
- too large for TJ, PT results only



PRITree Rendering Time Performance

TreeJuxtaposer renders **all** nodes for star trees

- branching factor k leads to O(k) performance



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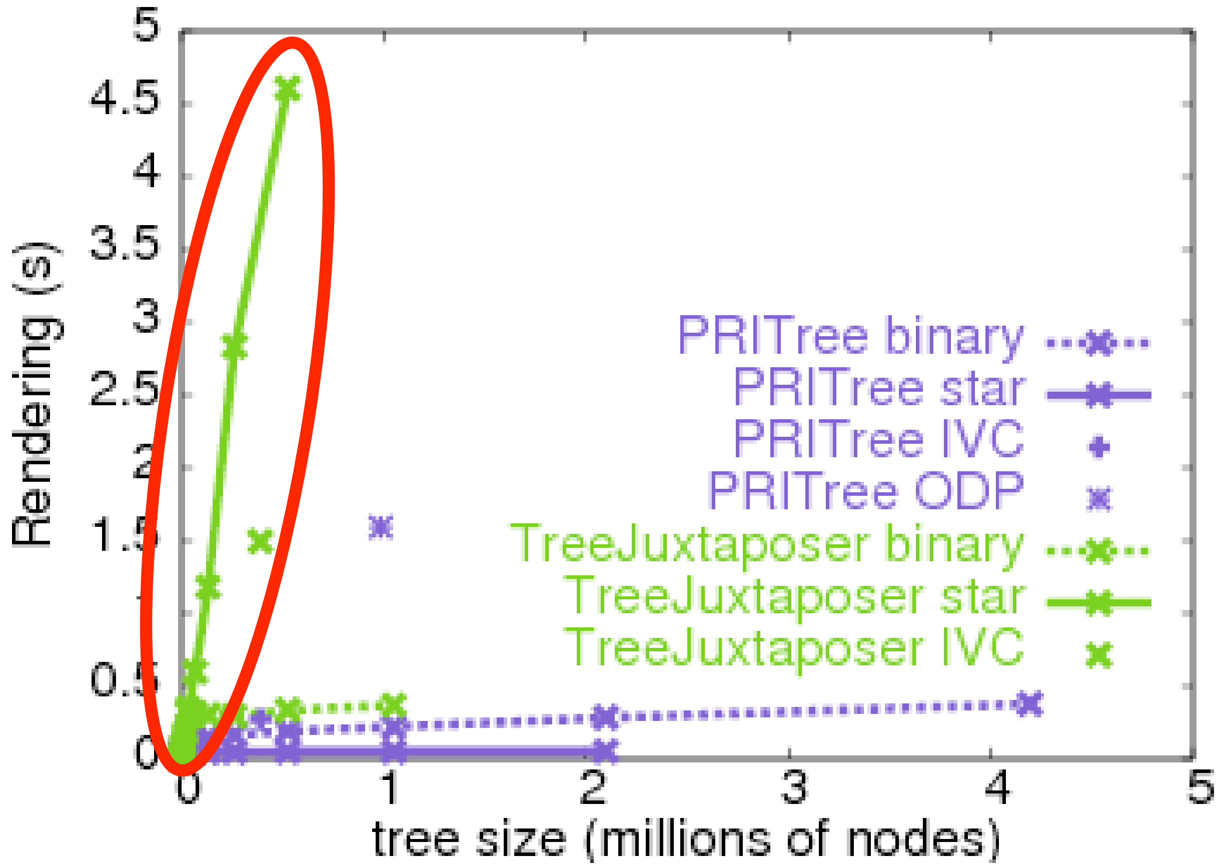
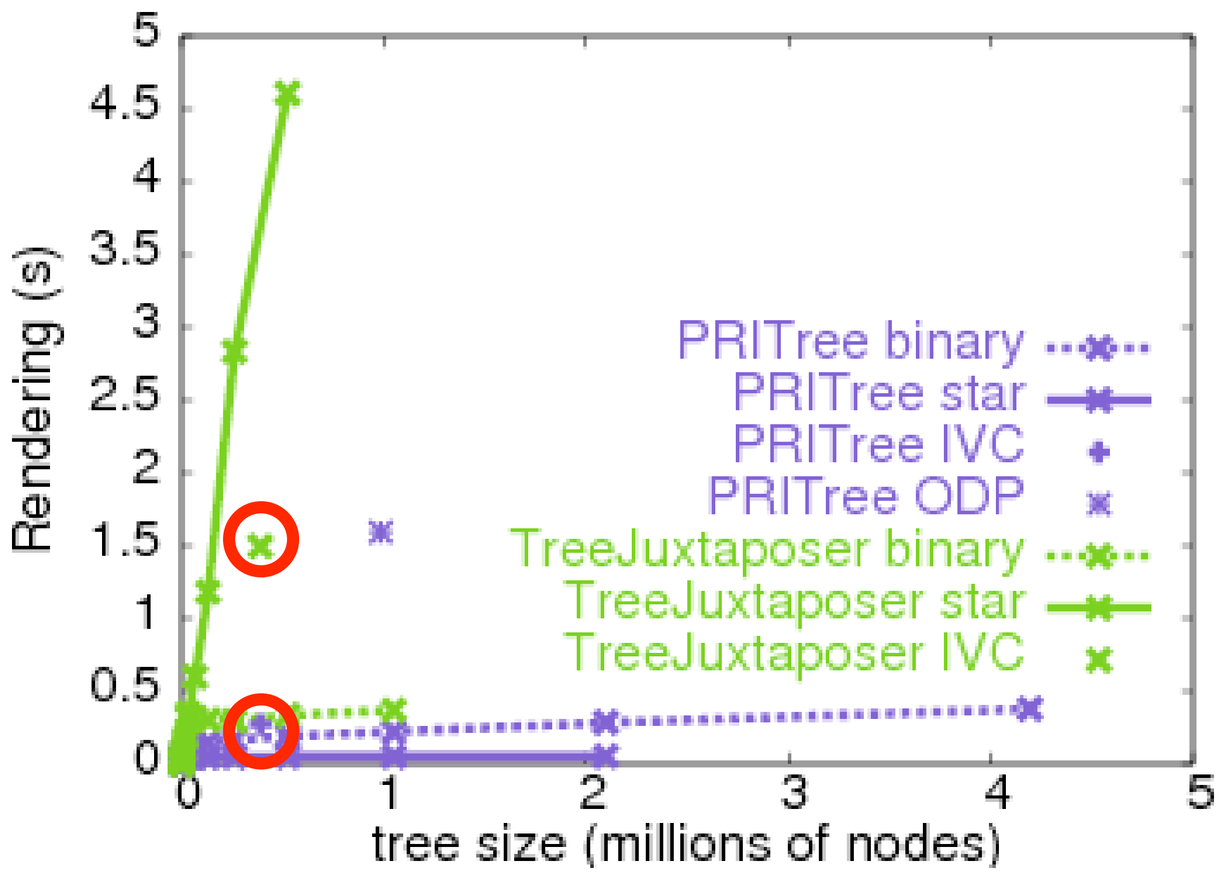


PRITree Rendering Time Performance

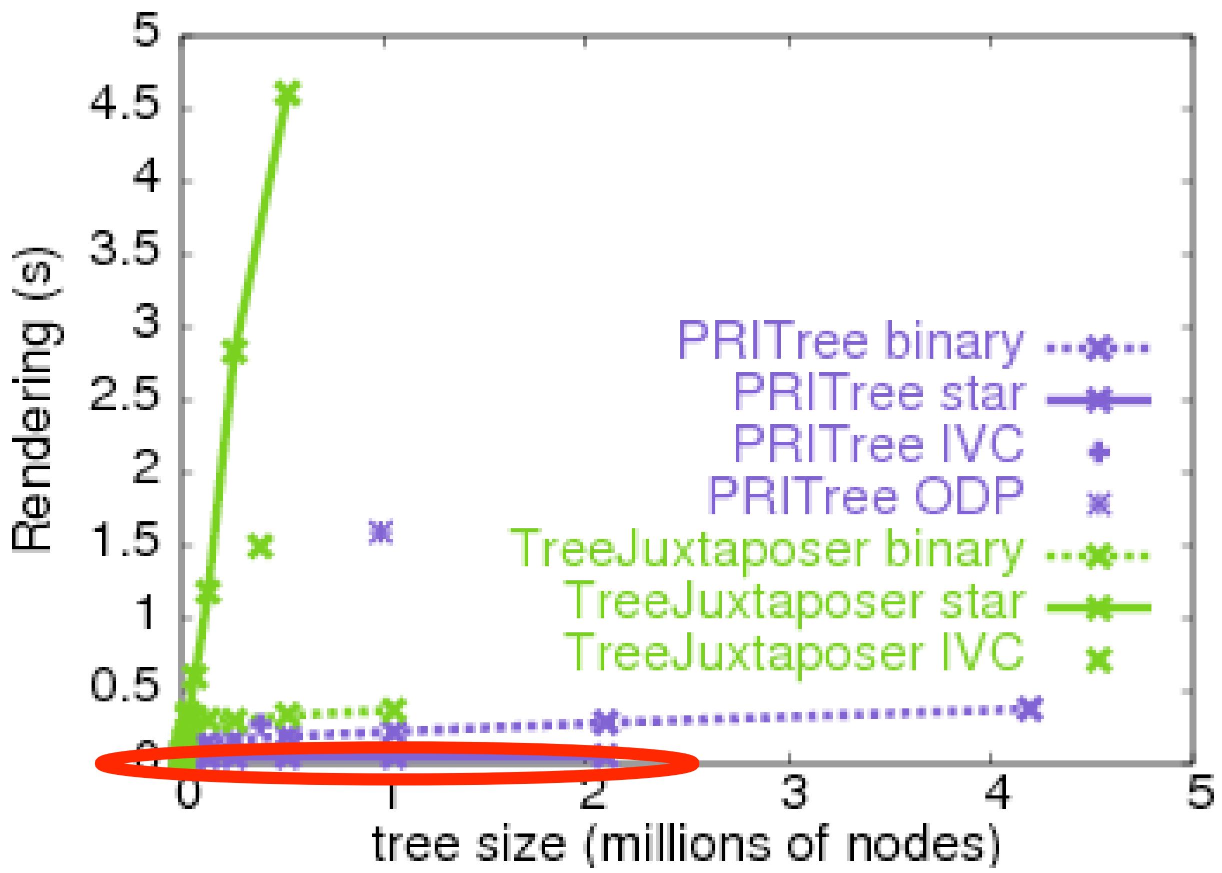
InfoVis 2003 Contest dataset

• 5x rendering speedup

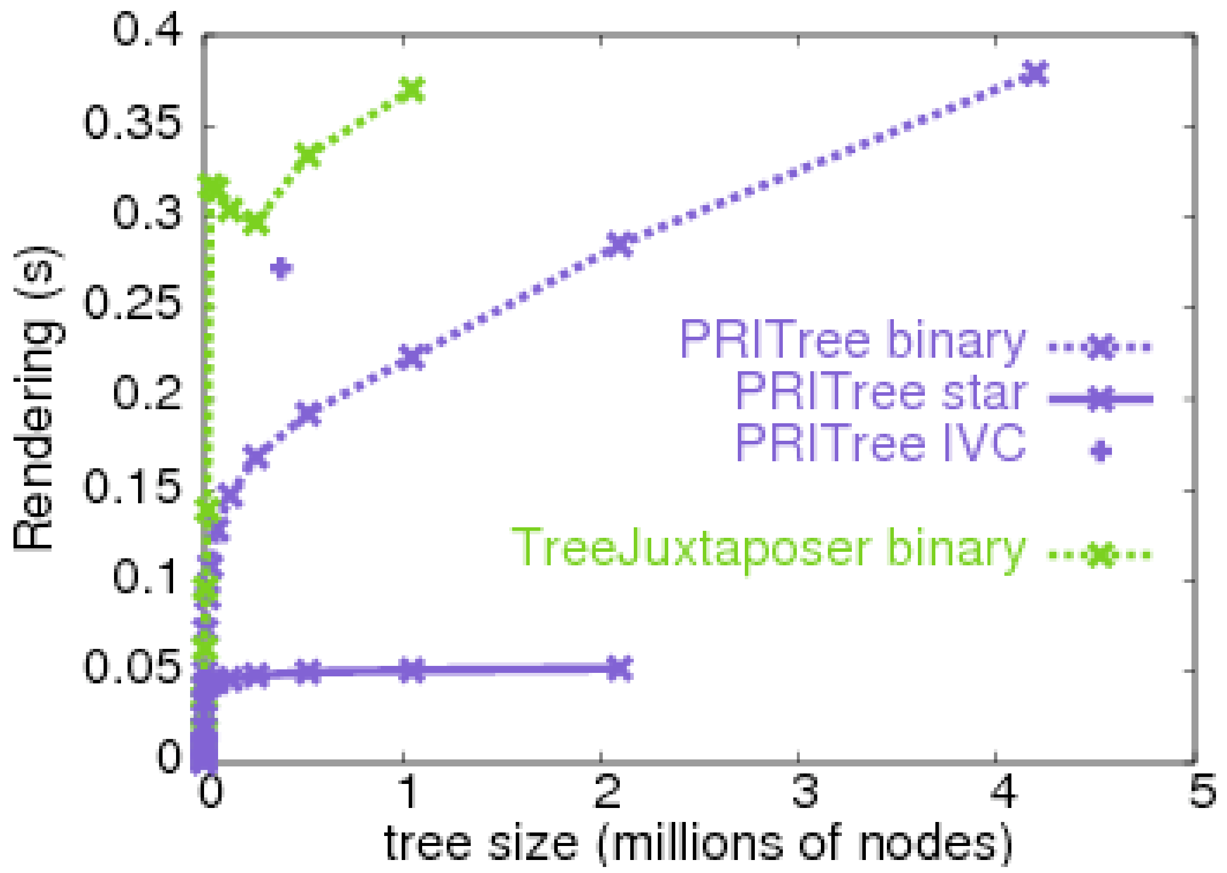


PRITree Rendering Time Performance

a closer look at the fastest rendering times



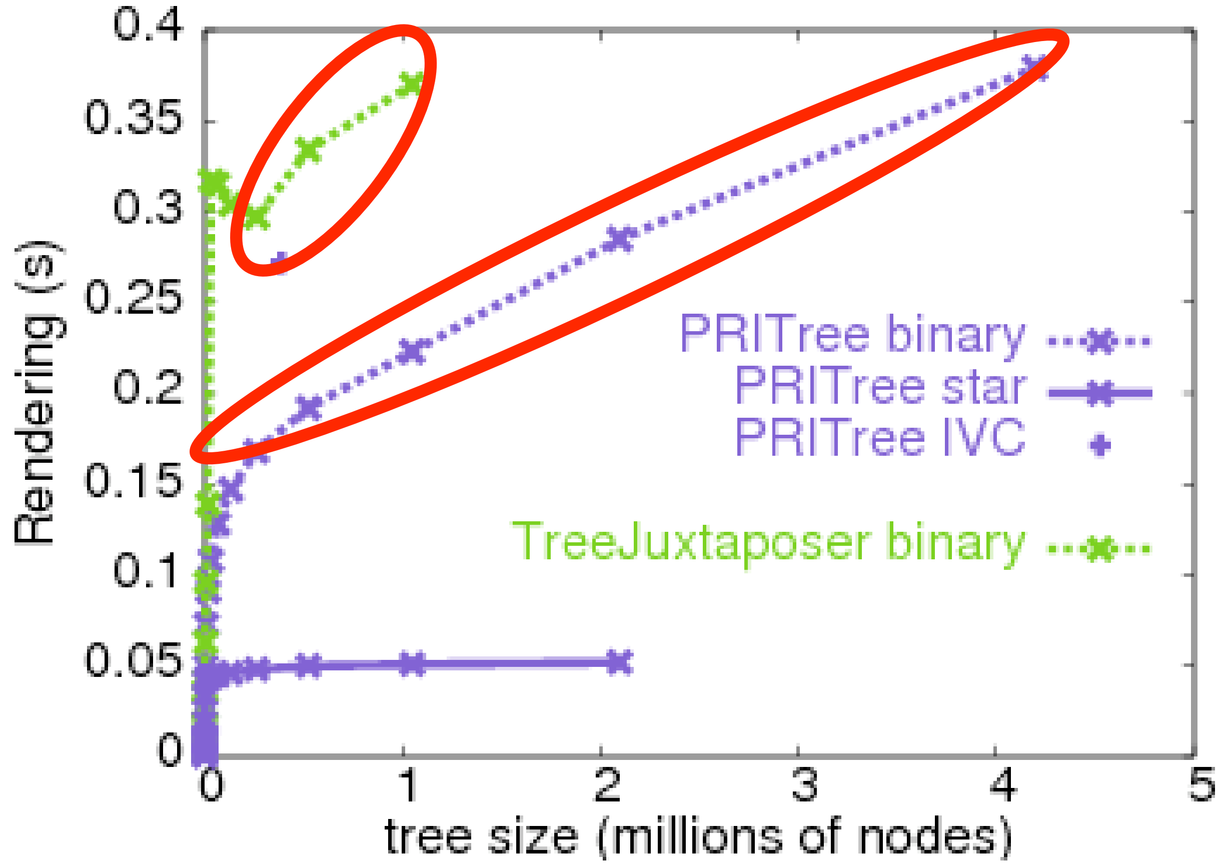
PRITree Rendering Time Performance



Detailed Rendering Time Performance

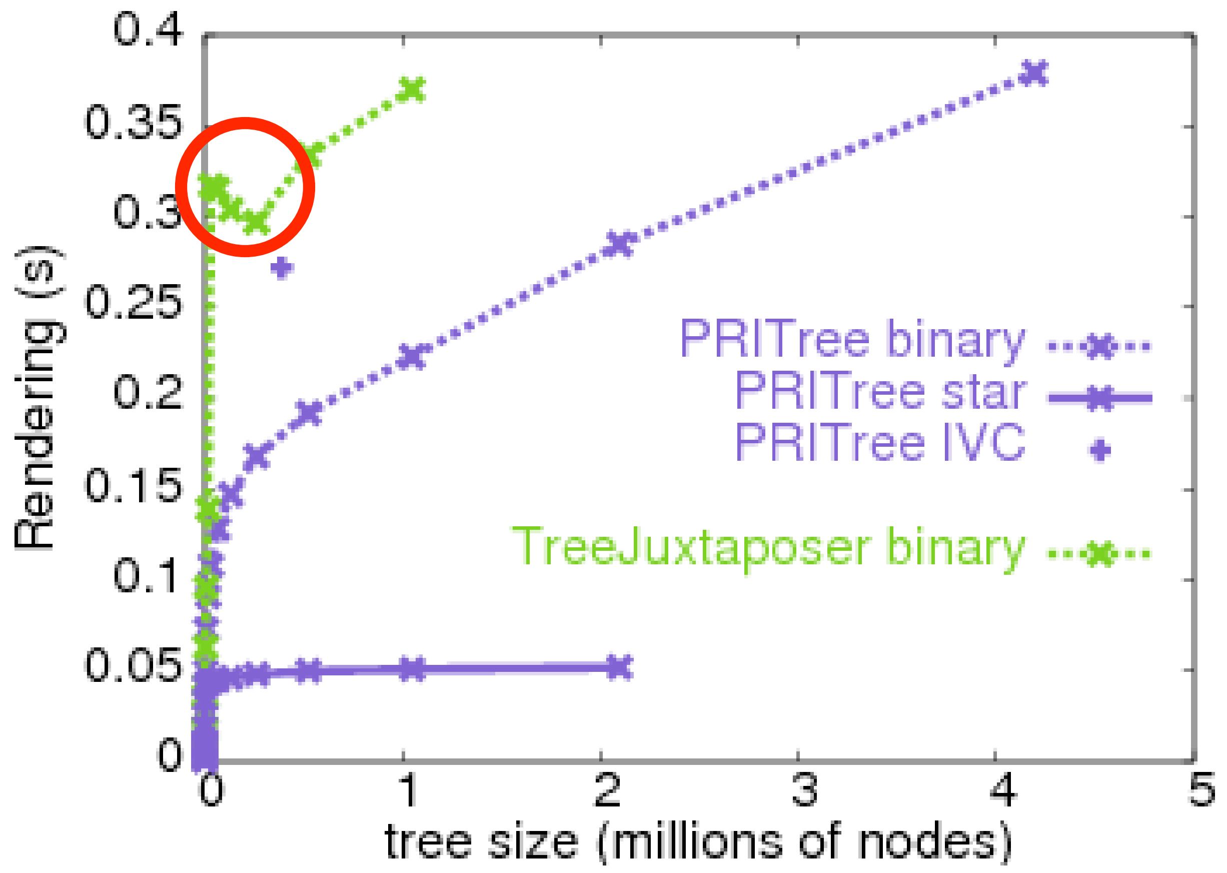
PRITree handles 4 million nodes in under 0.4 seconds

- TreeJuxtaposer takes twice as long to render 1 million nodes



Detailed Rendering Time Performance

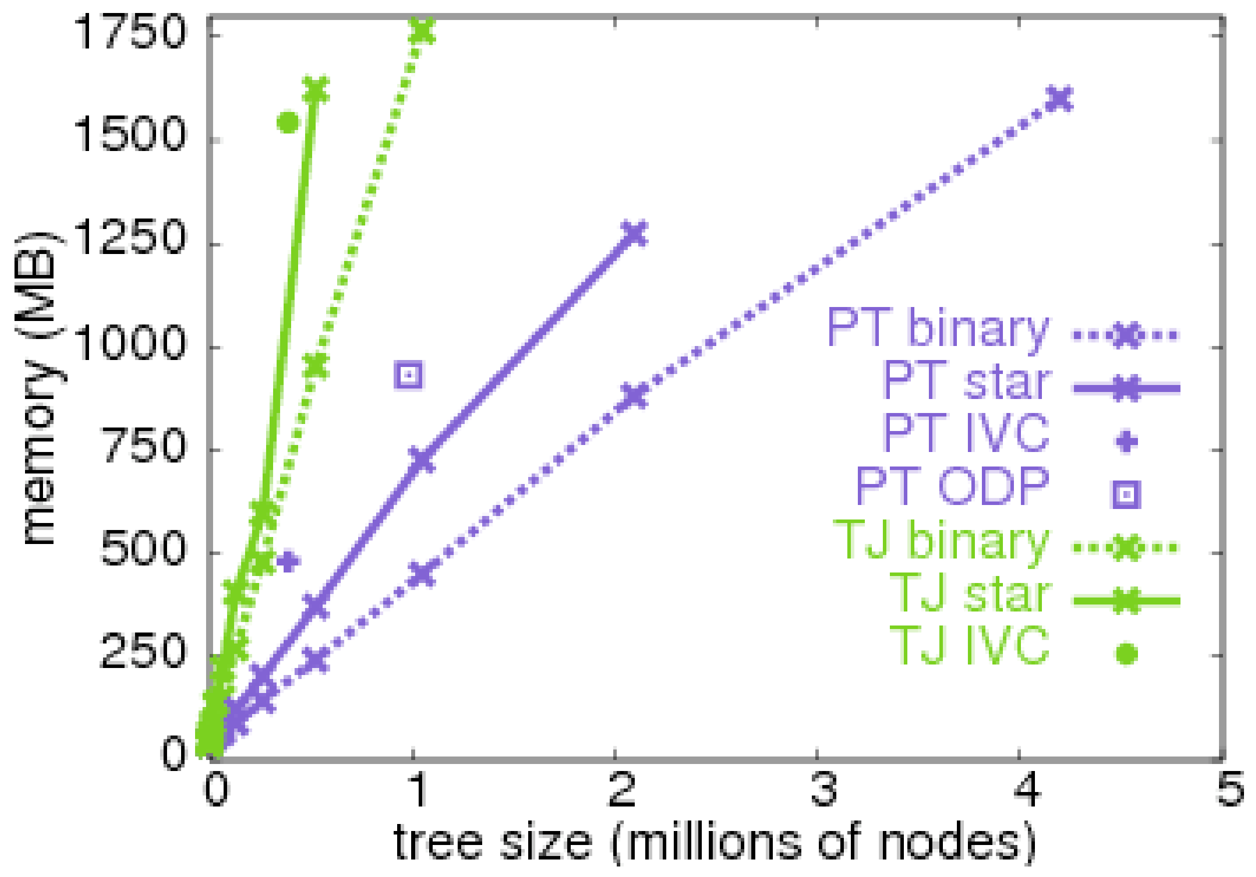
TreeJuxtaposer valley from overculling



Memory Performance

linear memory usage for both applications

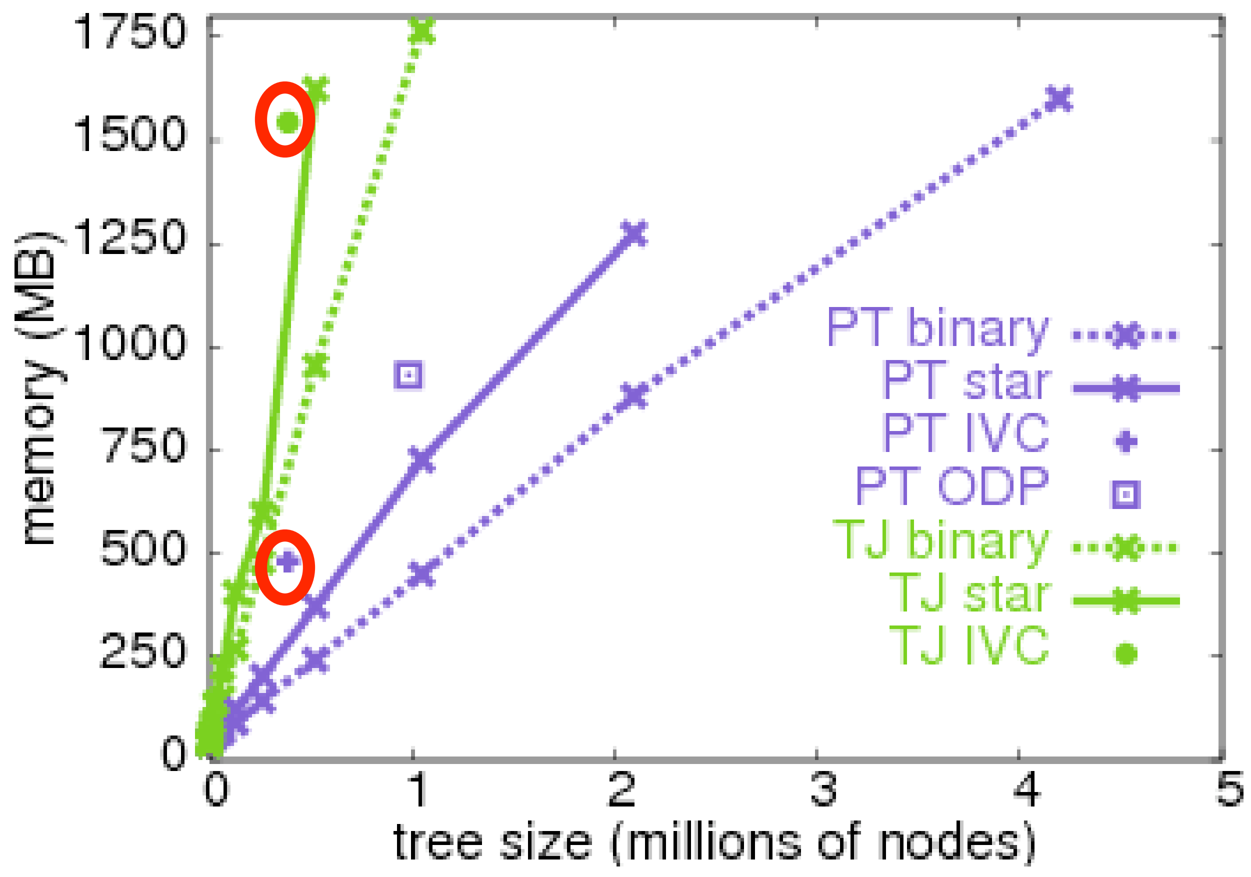
- 4-5x more efficient for synthetic datasets



Memory Performance

1GB difference for InfoVis contest comparison

- marked range storage changes improve scalability



Performance Comparison

- PRITree vs. TreeJuxtaposer
  - detailed benchmarks against identical TJ functionality
    - 5x faster, 8x smaller footprint
    - handles over 4M node trees
- PRISeq vs. SequenceJuxtaposer
  - 15x faster rendering, 20x smaller memory size
  - 44 species * 17K nucleotides = 770K items
  - 6400 species * 6400 nucleotides = 40M items

Future Work

- future work
  - editing and annotating datasets
  - PRISAD support for application specific actions
    - logging, replay, undo, other user actions
  - develop process or template for building applications

PRISAD Contributions

- infrastructure for efficient, correct, and generic accordion drawing
- efficient and correct rendering
  - screen-space partitioning tightly bounds overdrawing and eliminates overculling
- first generic AD infrastructure
  - PRITree renders 5x faster than TJ
  - PRISeq renders 20x larger datasets than SJ

Joint Work

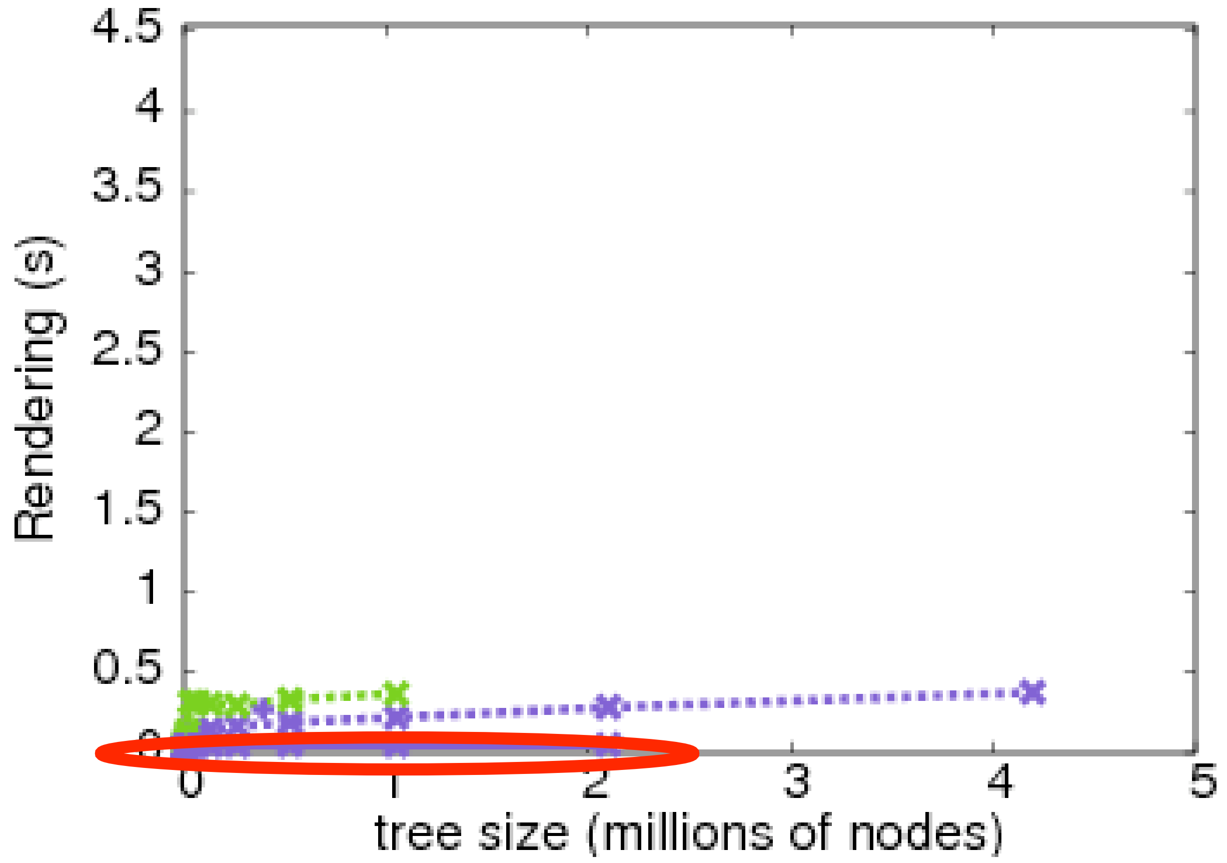
- TreeJuxtaposer
  - François Guimbretière, Serdar Ta_iran, Li Zhang, Yunhong Zhou
    - SIGGRAPH 2003
- SequenceJuxtaposer
  - James Slack, Kristian Hildebrand, Katherine St.John
    - German Conference on Bioinformatics 2004
- TJC/TJC-Q
  - Dale Beermann, Greg Humphreys
    - EuroVis 2005
- PRISAD
  - James Slack, Kristian Hildebrand
    - IEEE InfoVis Symposium 2005
    - Information Visualization journal, to appear

Open Source

- software freely available from http://olduvai.sourceforge.net
  - SequenceJuxtaposer olduvai.sf.net/sj
  - TreeJuxtaposer olduvai.sf.net/tj
  - requires Java and OpenGL
    - JOGL bindings for TJ, GL4Java for SJ (JOGL coming soon)
- papers, talks, videos also from http://www.cs.ubc.ca/~tmm

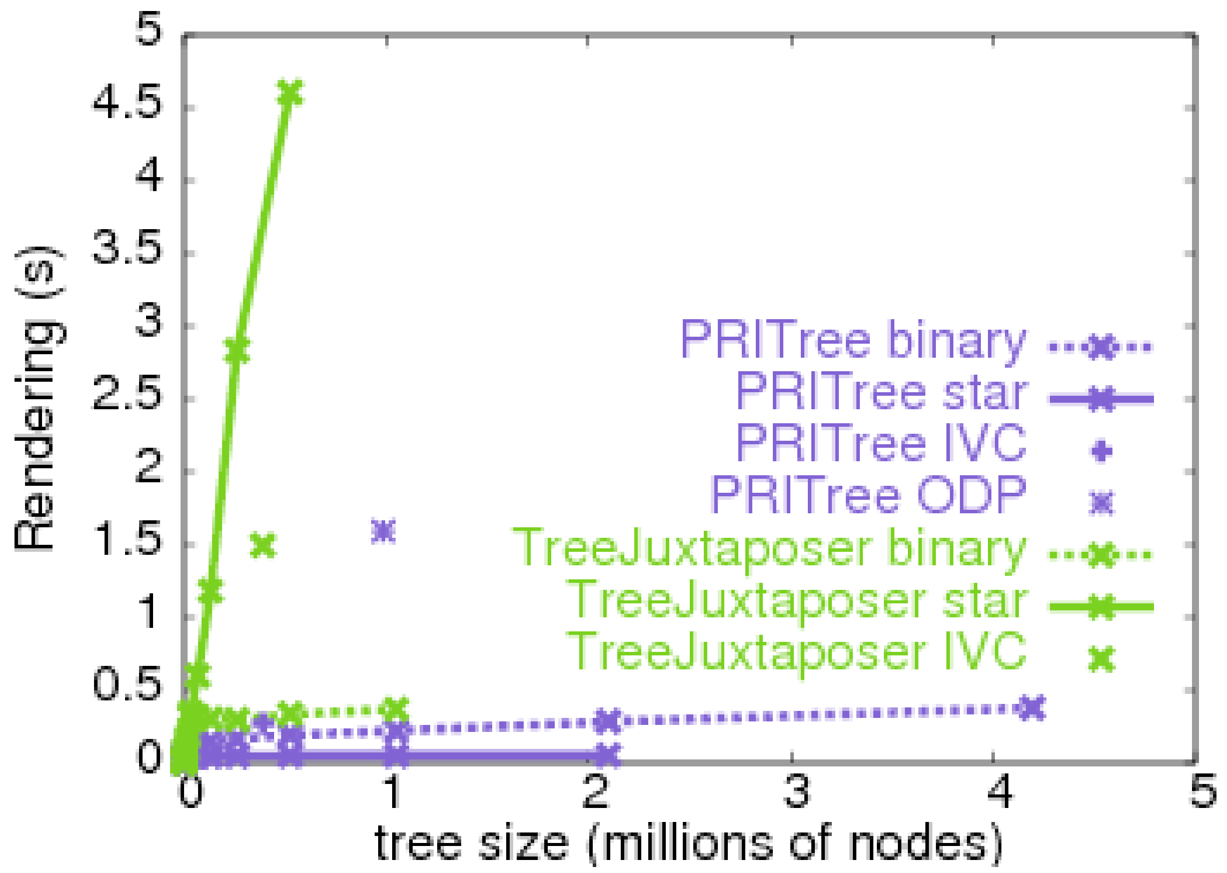
PRITree Rendering Time Performance

a closer look at the fastest rendering times



PRITree Rendering Time Performance

a closer look at the fastest rendering times


Rendering (s)
tree size (millions of nodes)
PRITree binary
PRITree star
PRITree IVC
PRITree ODP
TreeJuxtaposer binary
TreeJuxtaposer star
TreeJuxtaposer IVC