Getting the Most Out of *SnB*

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Hauptman-Woodward Med. Res. Inst.

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Overview

- *Shake-and-Bake*
  - Direct Methods Optimization Technique
  - Multiple Trial Structures
  - Real Space ⇔ Reciprocal Space
- *SnB* is the program based on *Shake-and-Bake*
- Phase Refinement Techniques
  - Parameter Shift
  - Tangent Formula
  - Simulated Annealing
  - Genetic Algorithms

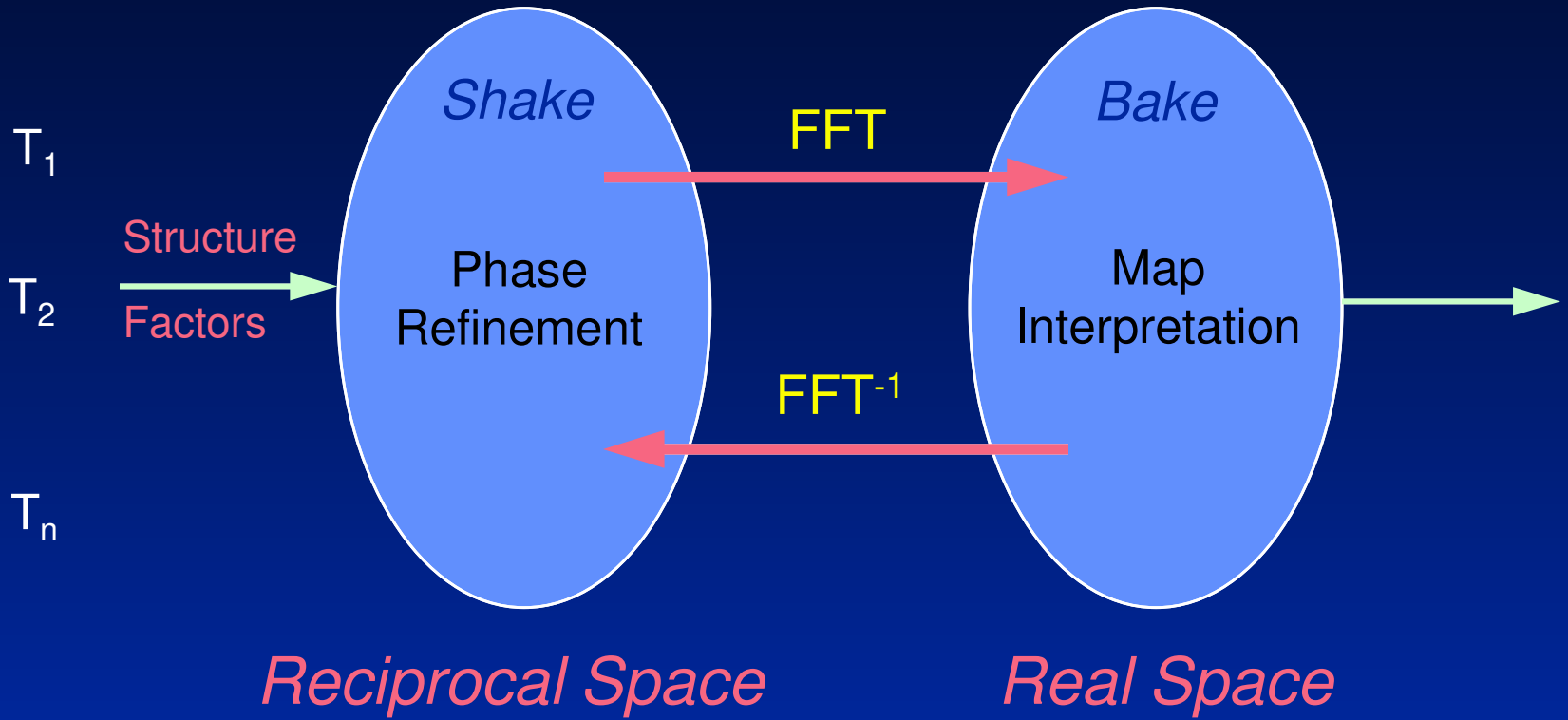
Computing Platforms

- Unix Workstations
  - SGI
  - Sun
  - DEC/Alpha
  - IBM RS6000
- Thinking Machines Corp. CM-5
- Cray T3D
- Cray C90
- IBM SP2

Availability of *SnB*

- MSC's teXsan 1-7.2
- MacScience
- Pittsburgh Supercomputing Center
- Hauptman-Woodward Inst.
- Cornell Theory Center

Shake-and-Bake



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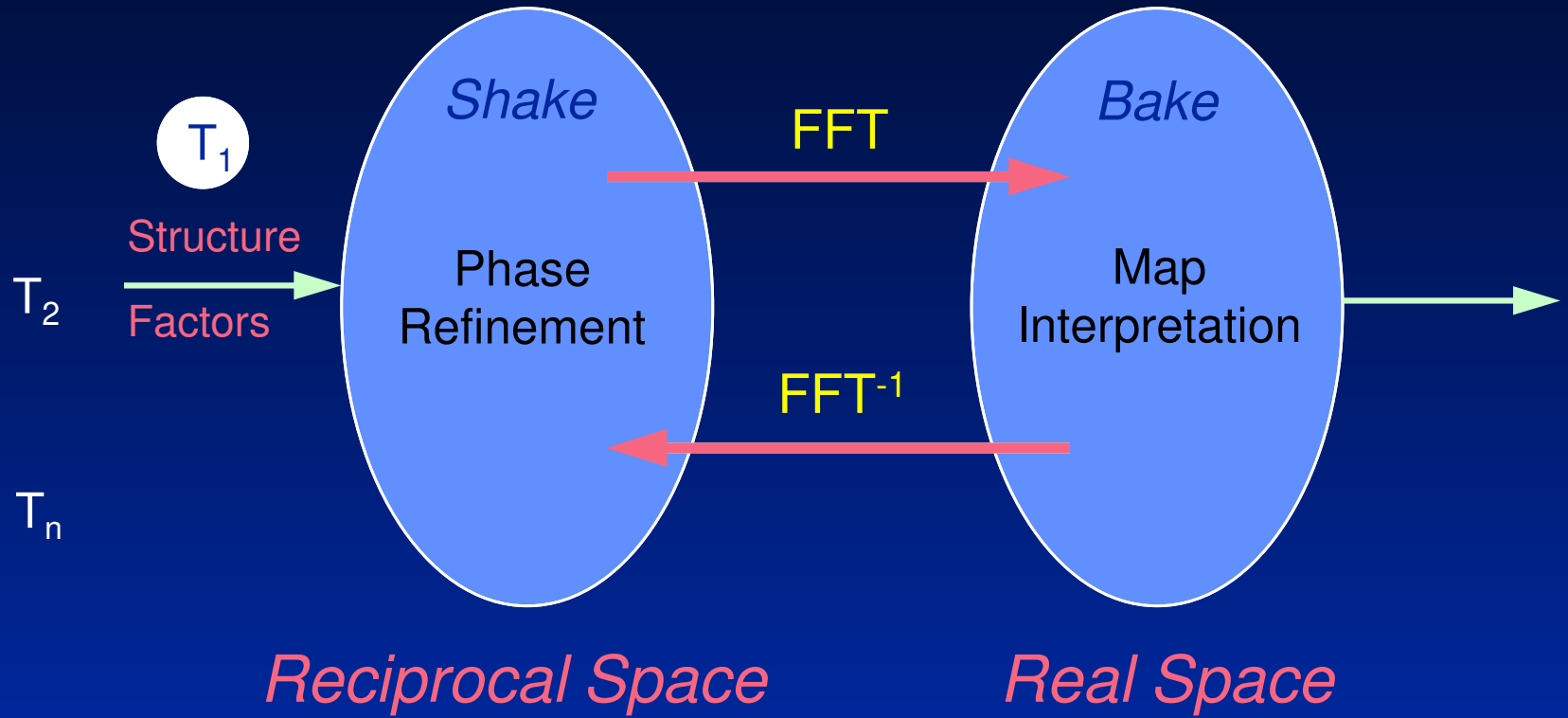

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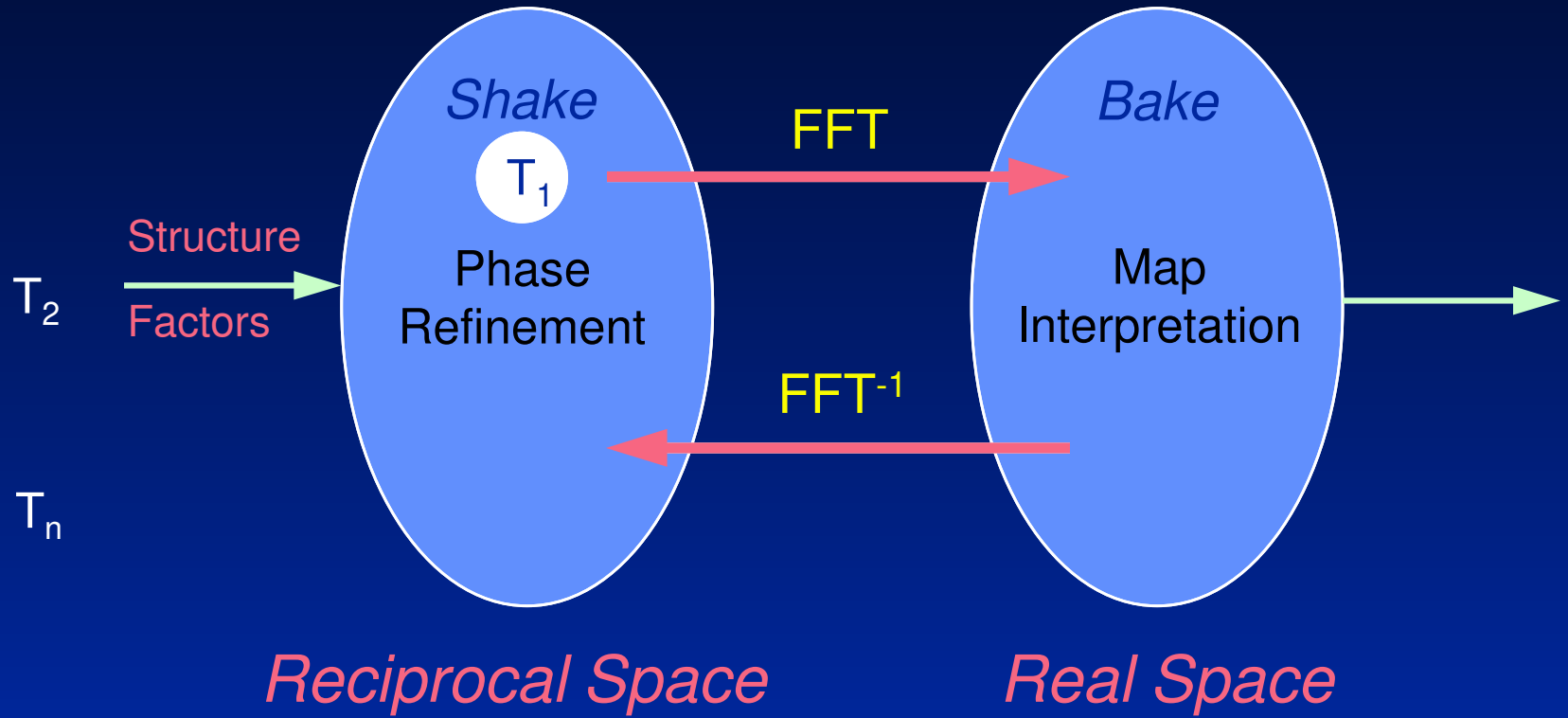

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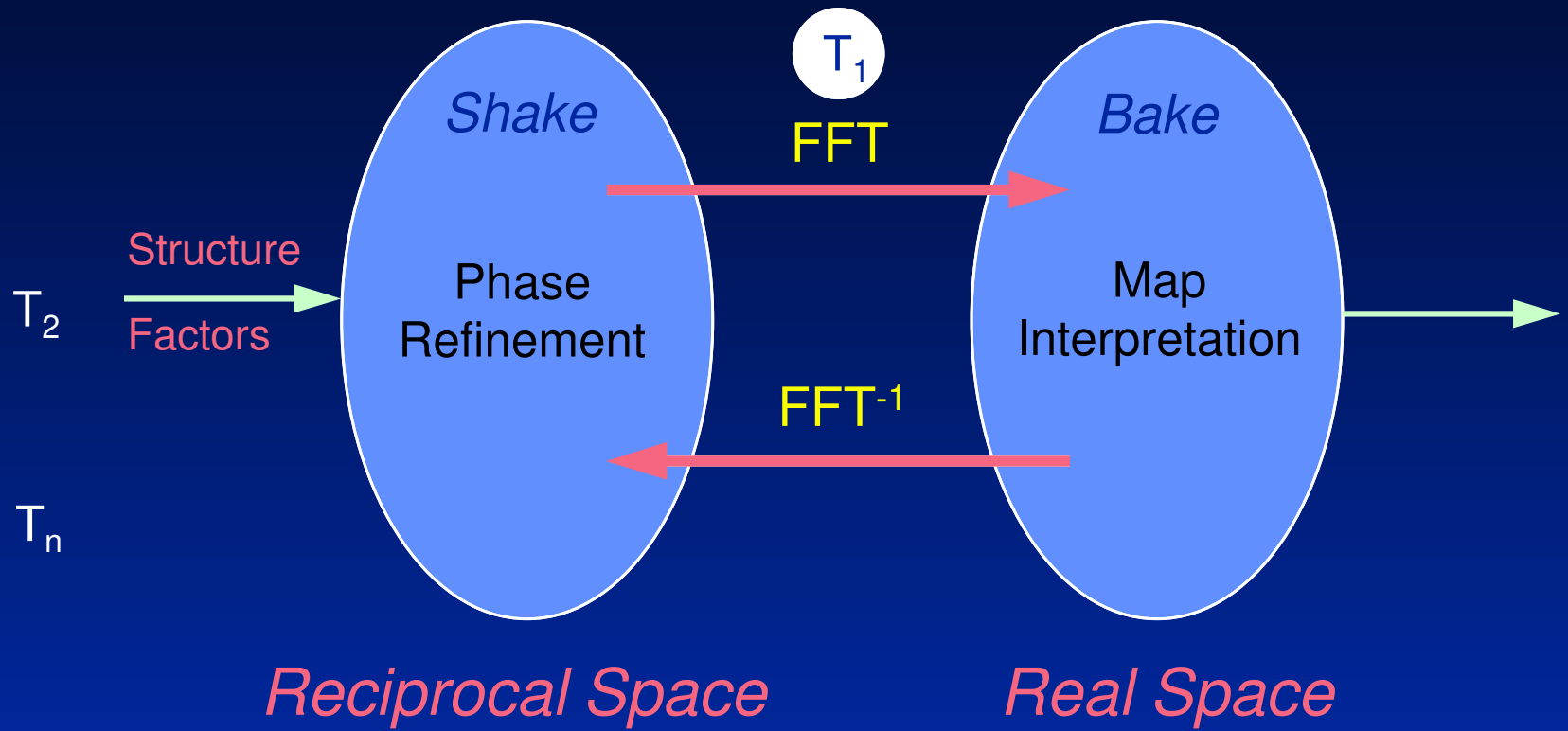

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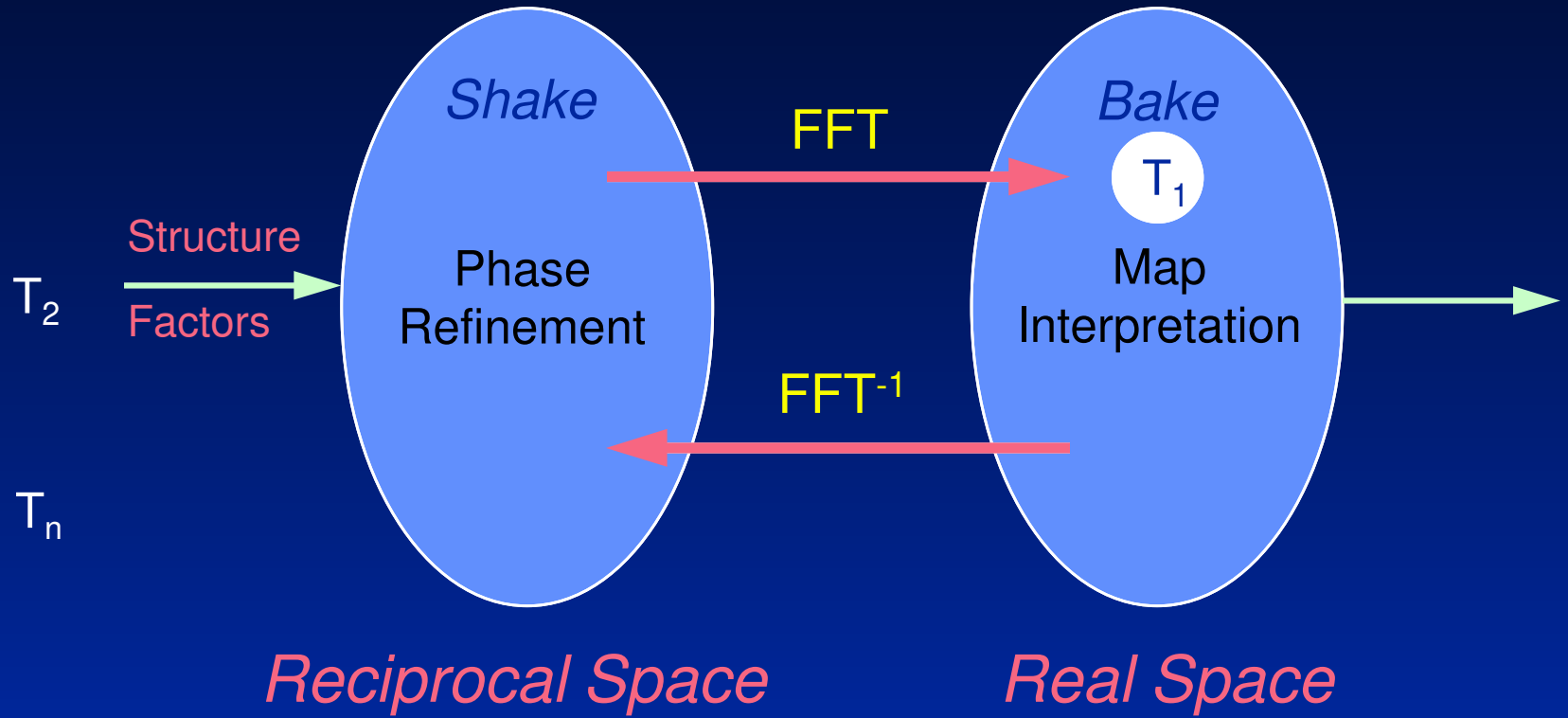

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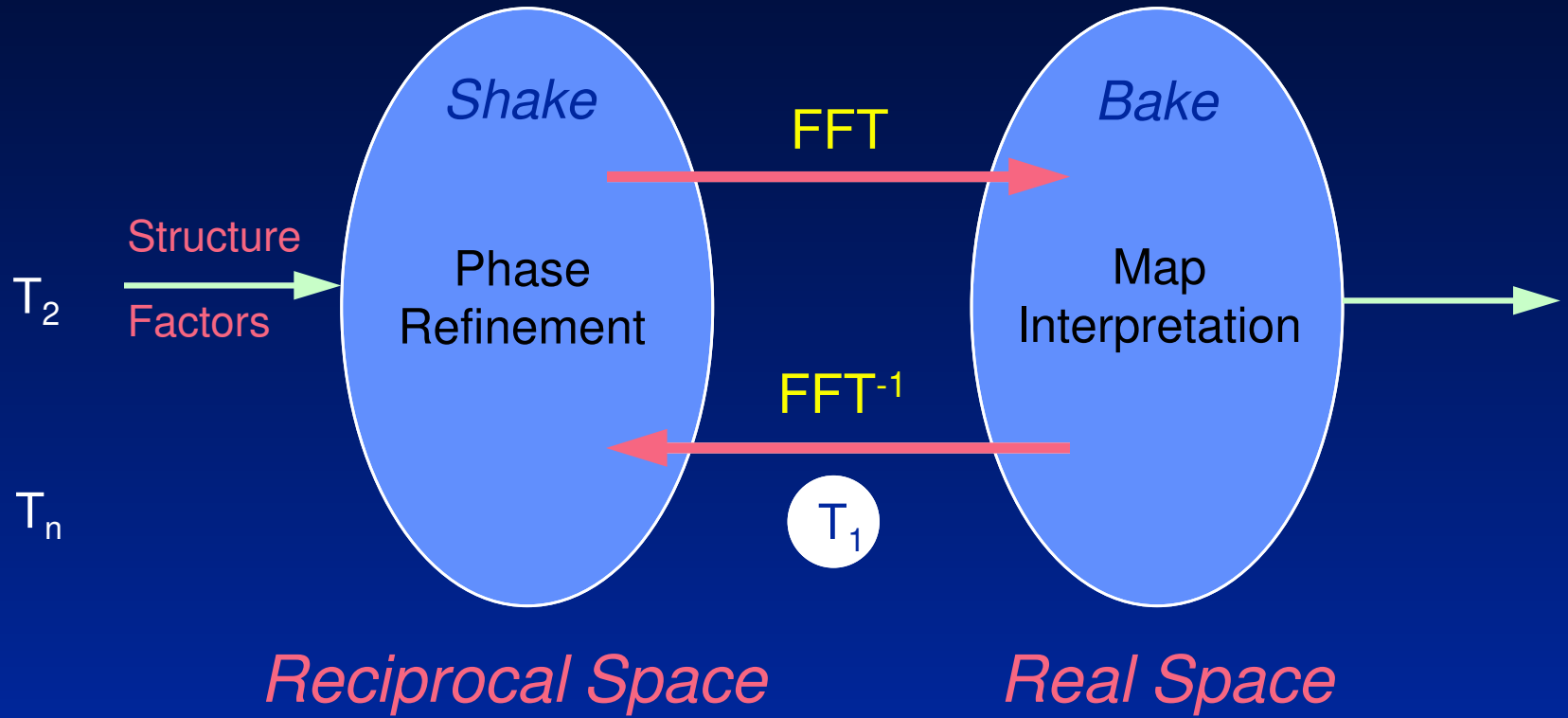

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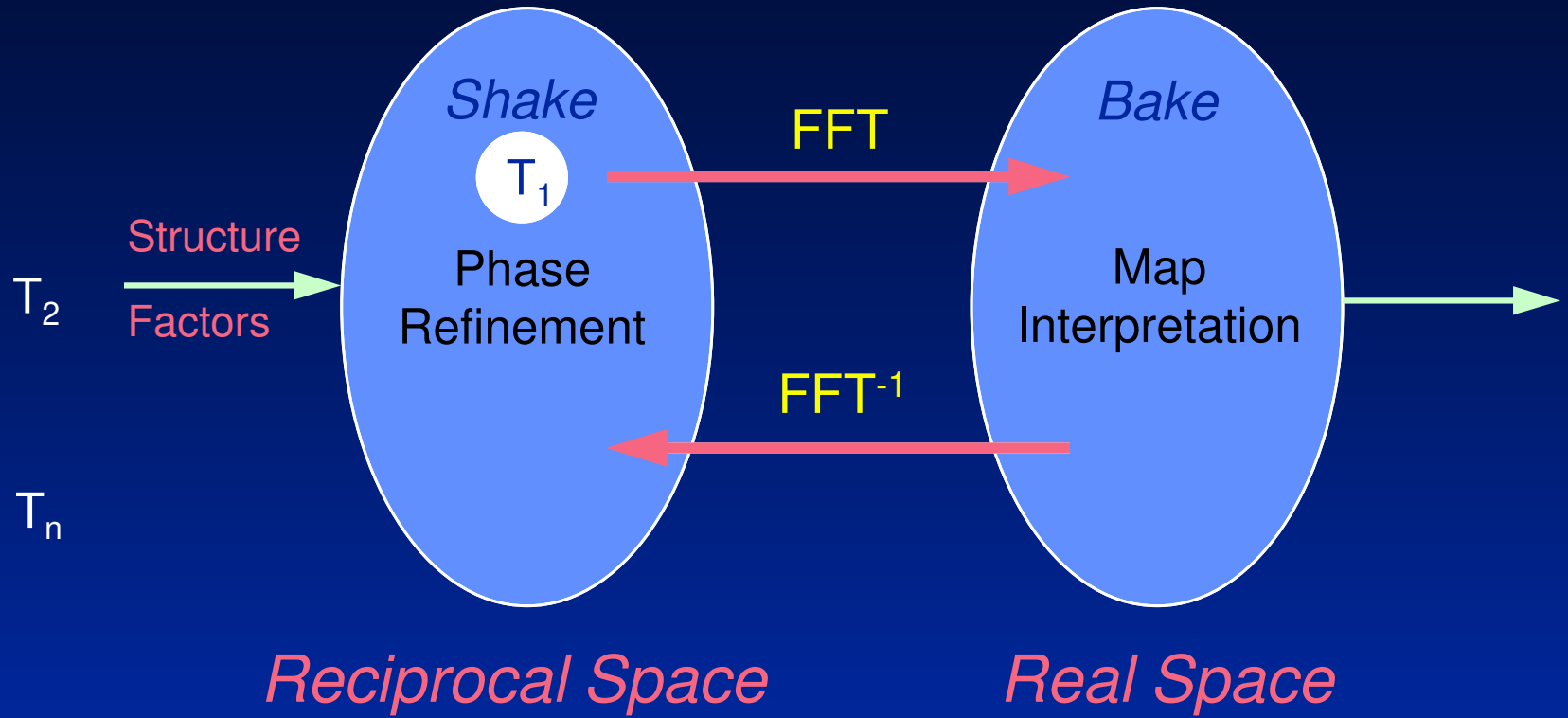

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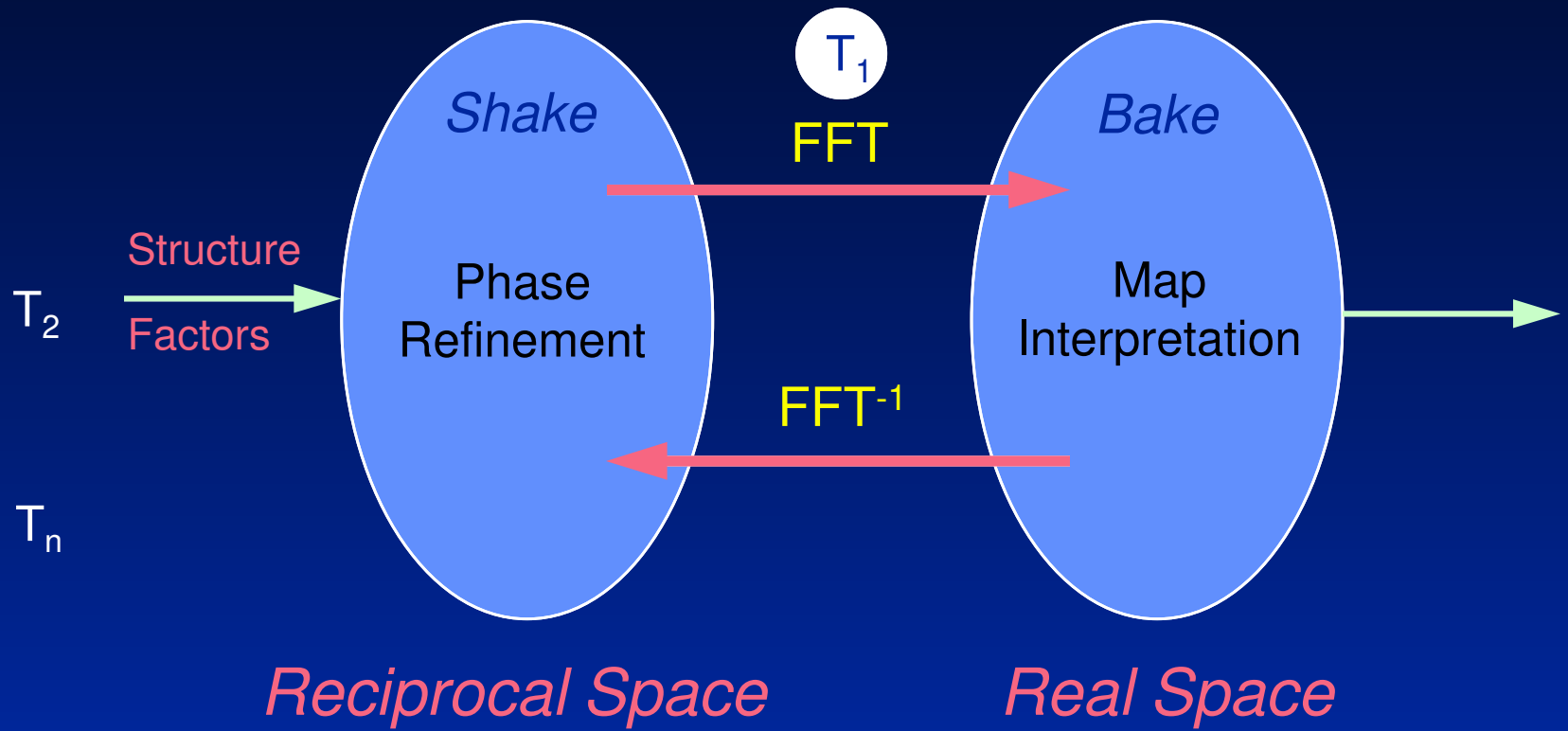

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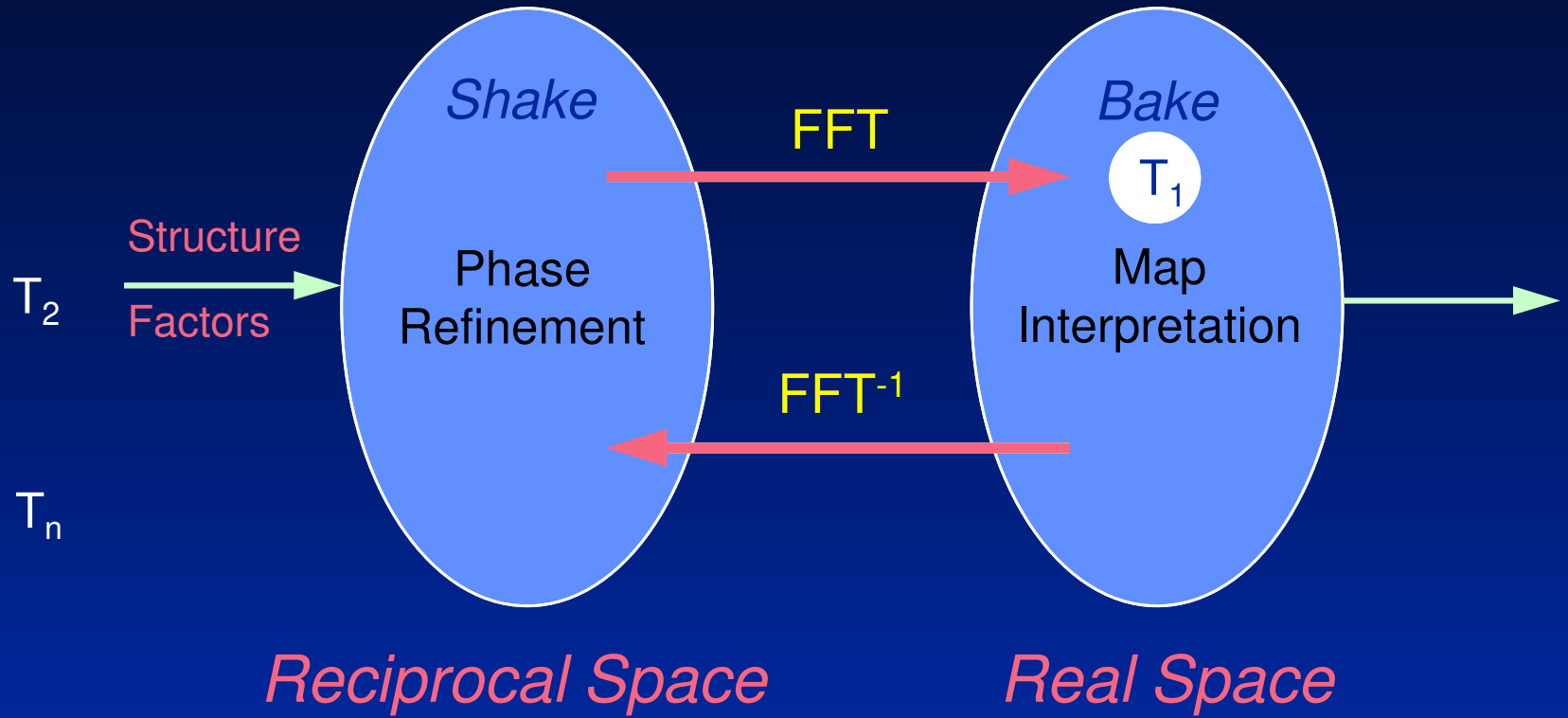

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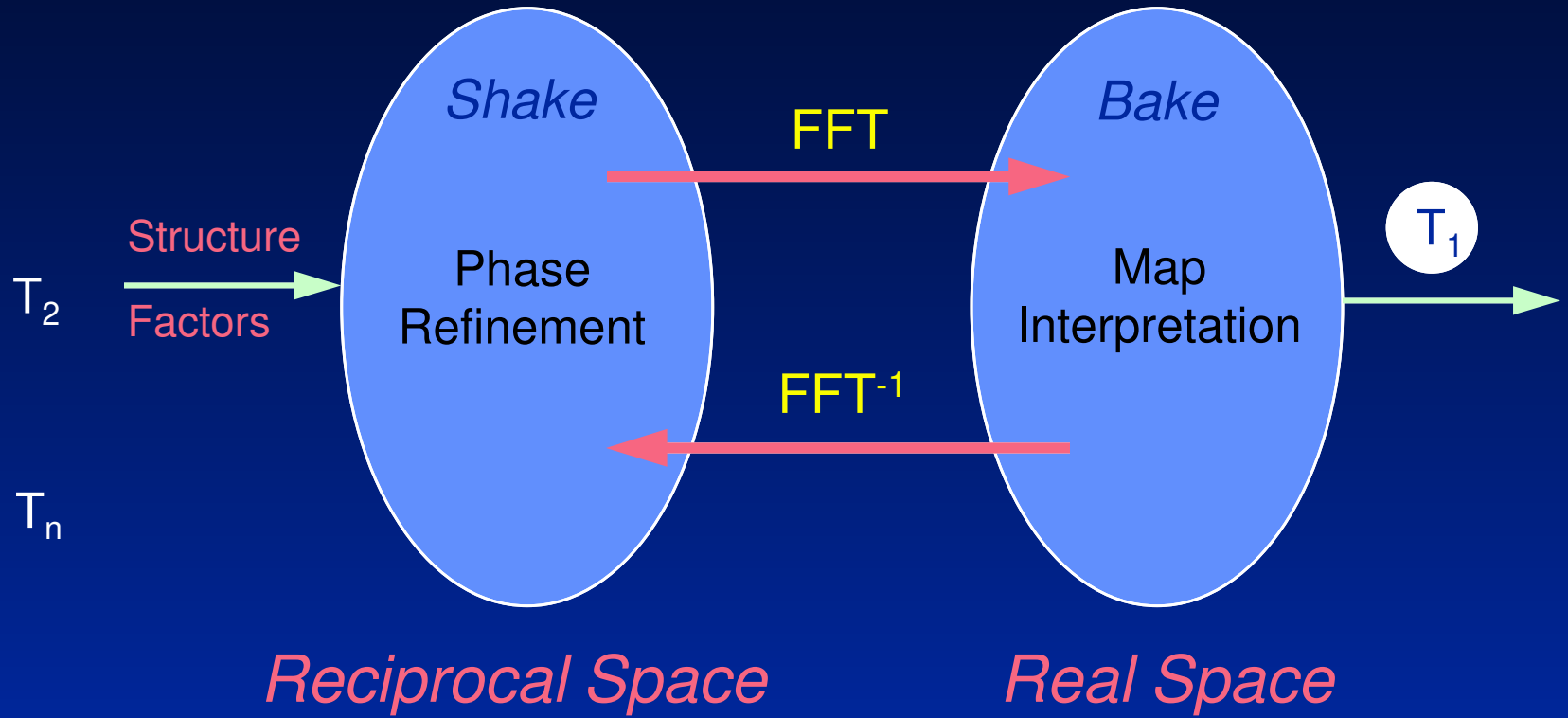

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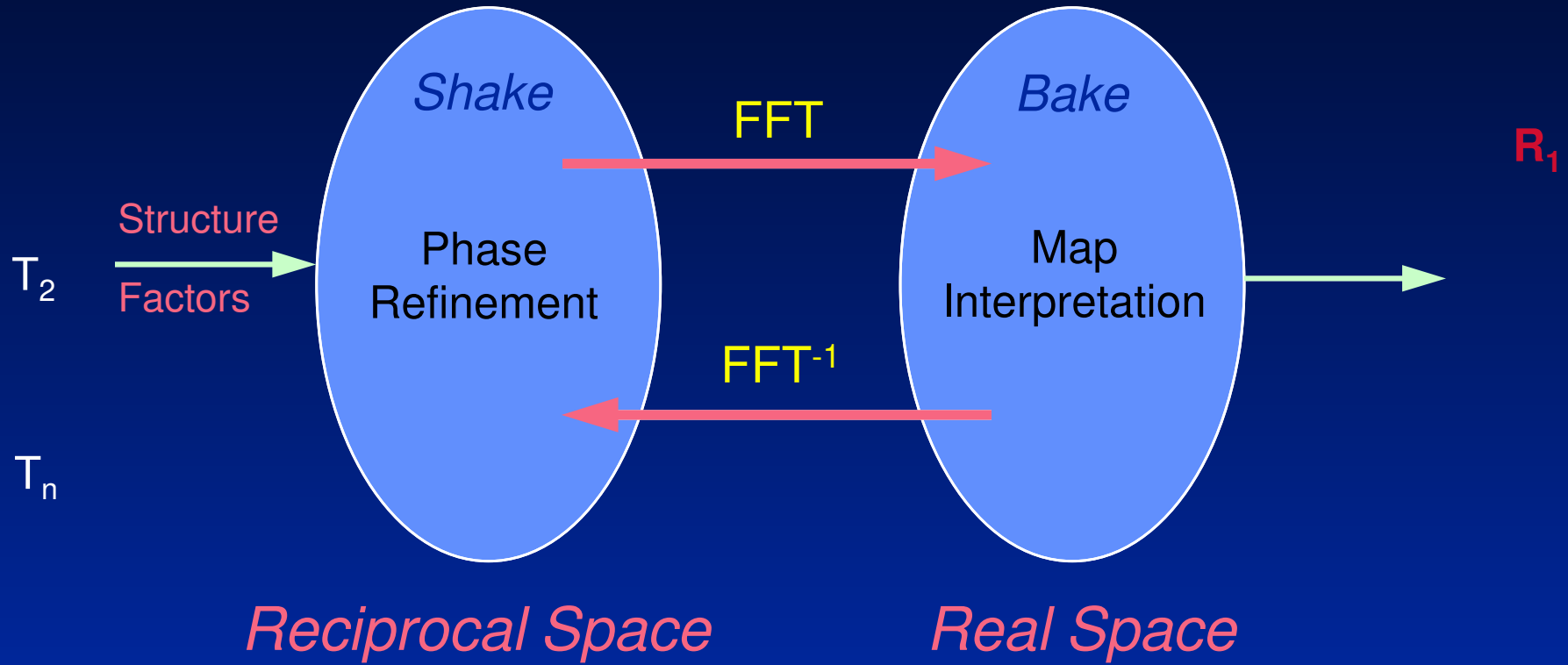

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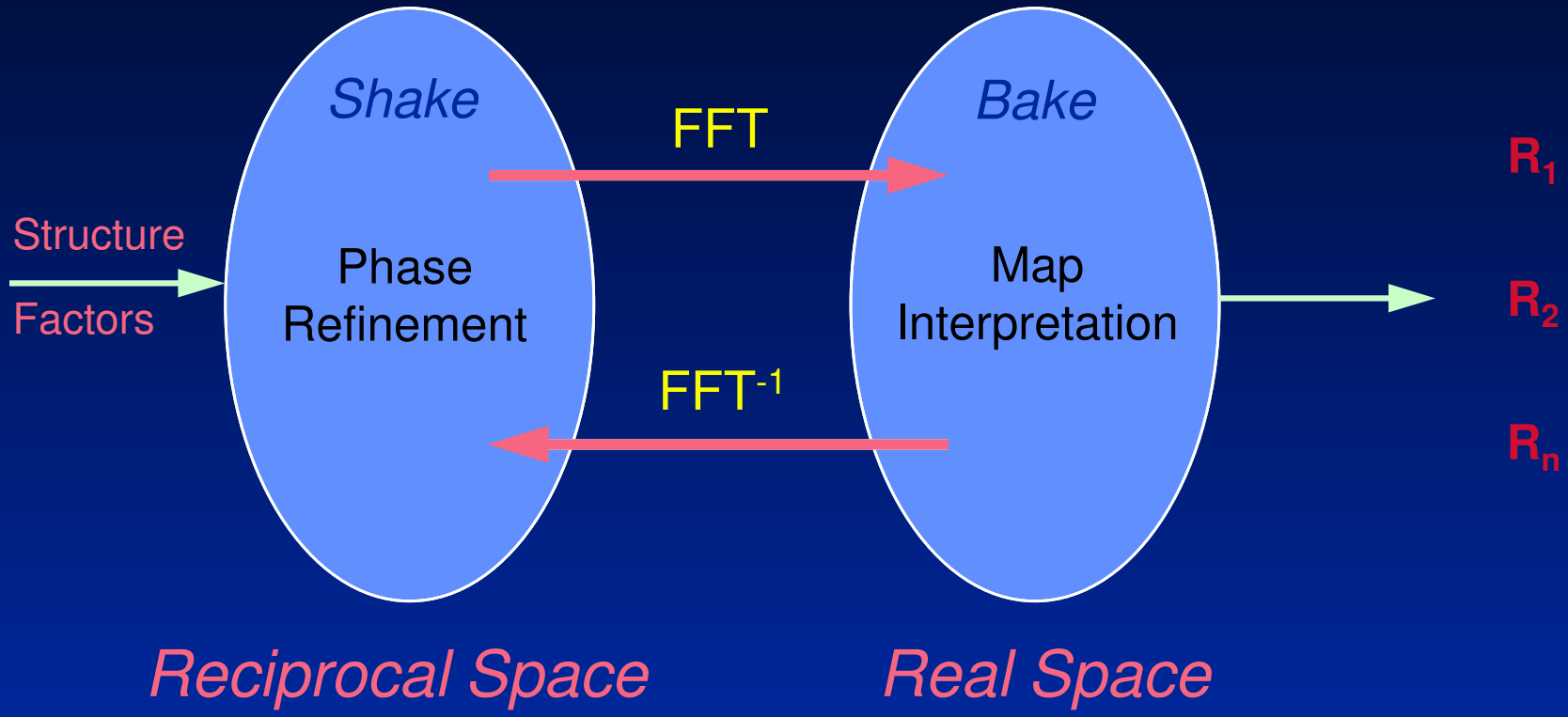
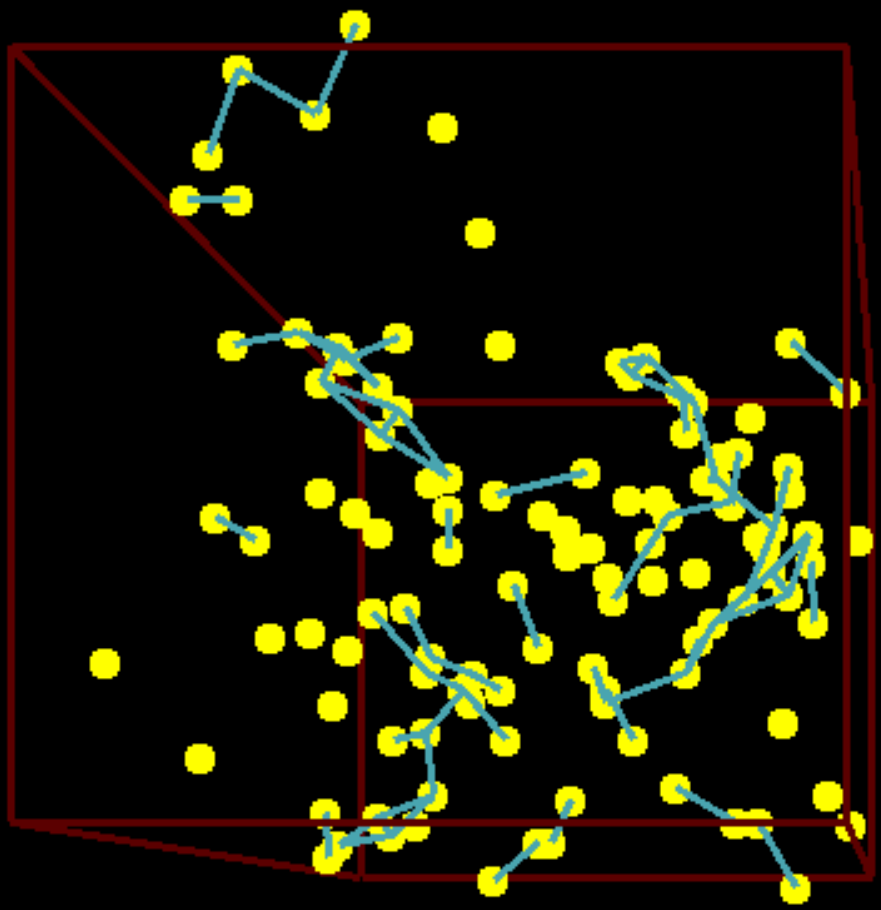
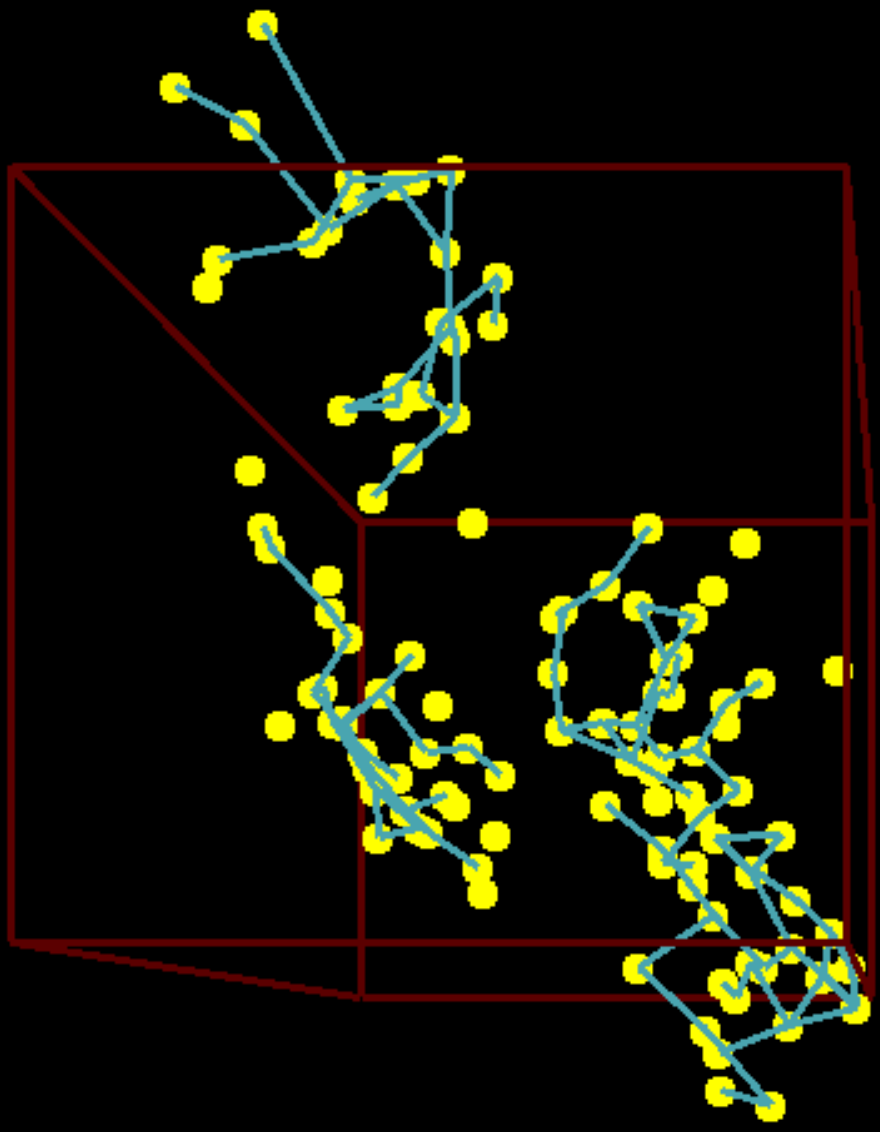
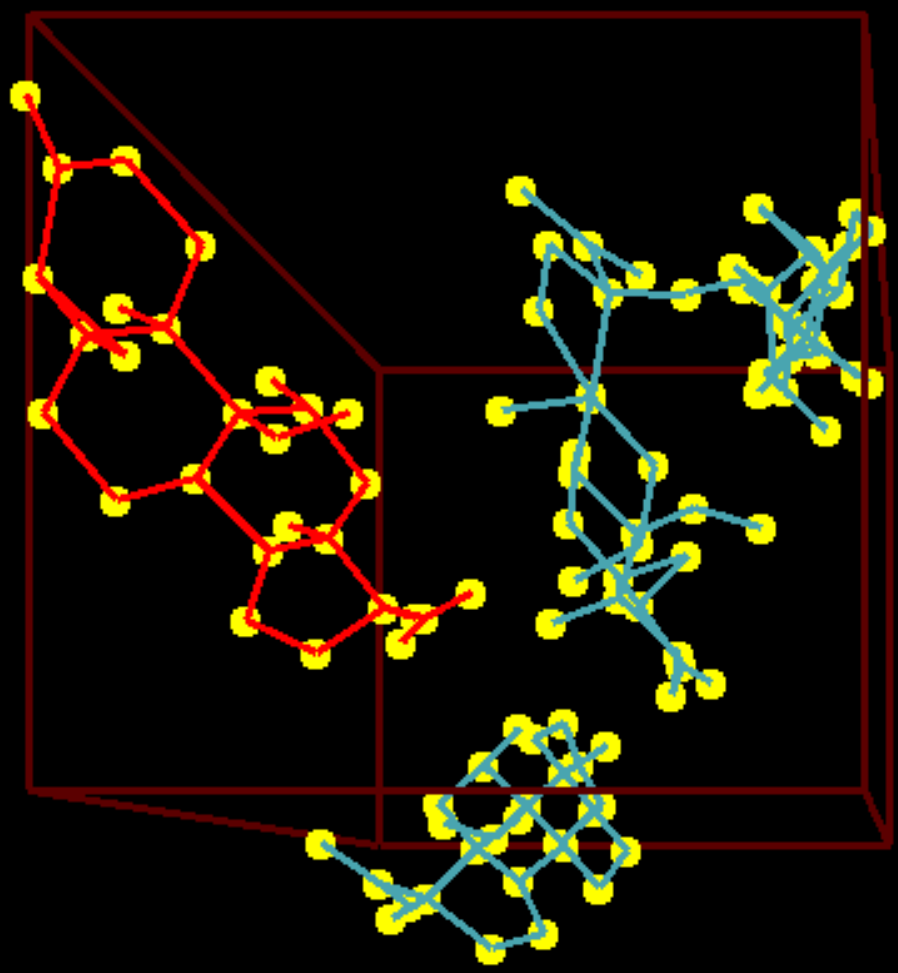
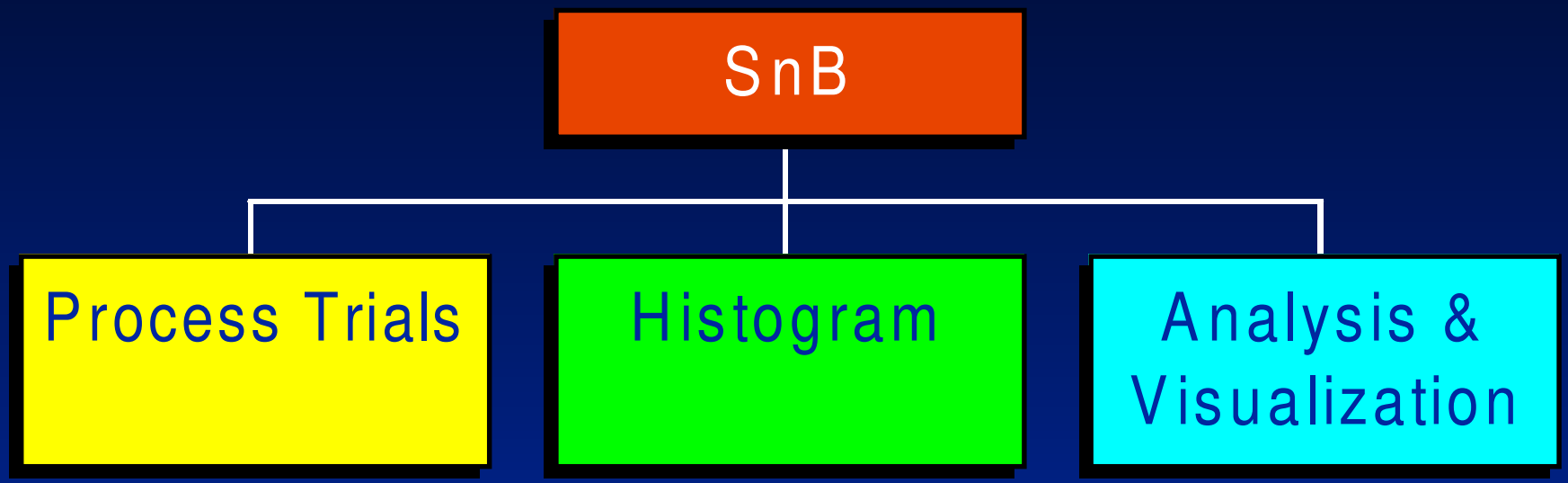


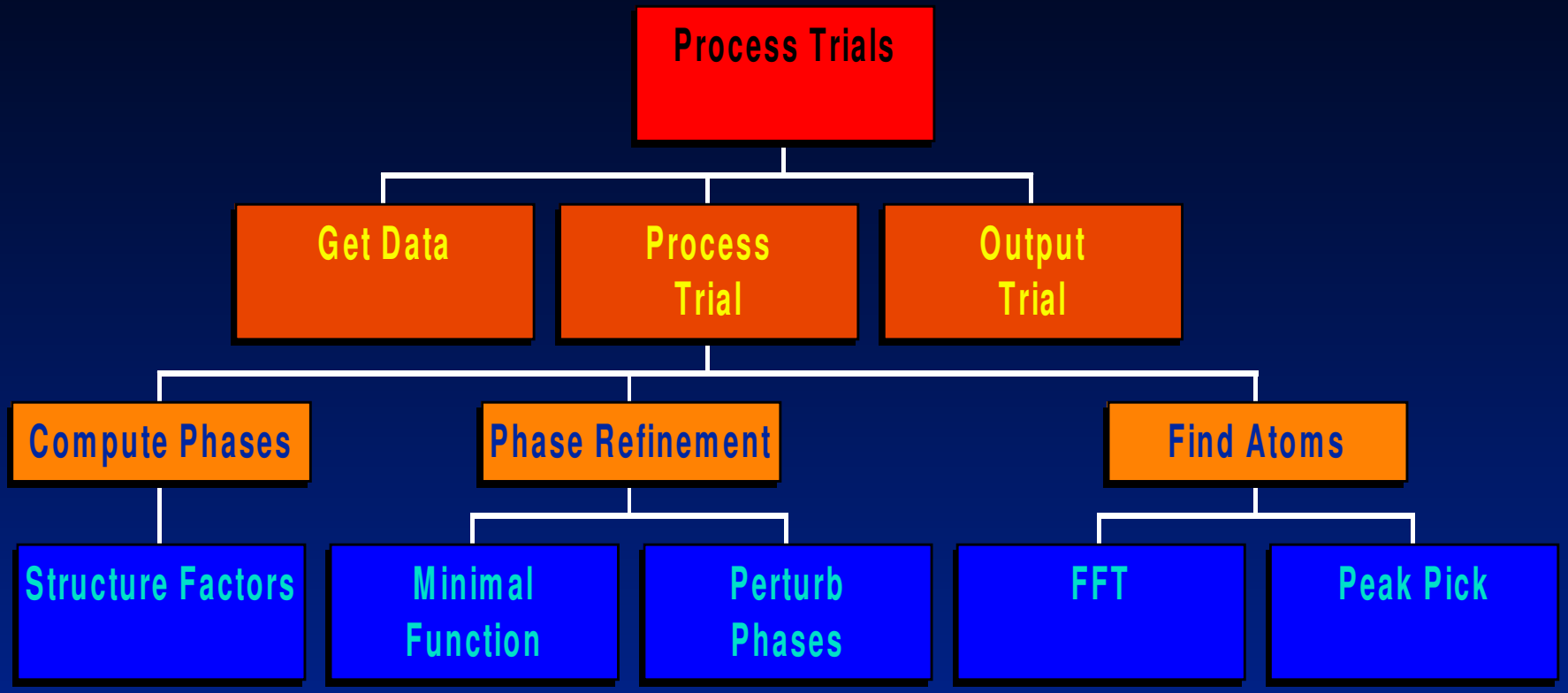






Structure of *SnB*




Process Trials
Get Data
Process Trial
Output Trial
Compute Phases
Phase Refinement
Find Atoms
Structure Factors
Minimal Function
Perturb Phases
FFT
Peak Pick

SnB Default Parameters

Atoms in asymmetric unit	n
Number of Phases	$8n$ - $10n$
Number of Triples	$70n$ - $100n$
Number of Quartets	0
Number of Cycles (Parameter Shift, Cent. Search)	$n/2$
Number of Cycles (Tangent Refinement)	$n/4$
E-Fourier Recycling Steps	C

Crambin

Atoms in asymmetric unit	*400*
Number of Phases	4,000
Number of Triples	40,000
Number of Quartets	0
Number of Cycles (Parameter Shift)	*200*
E-Fourier Recycling Steps	*5*

Structures

Structure	*Atoms*	*Space Group*	*Success Rate*
Ternatin	**110**	**$P2_12_12_1$**	**2%**
Scripps	**144**	**P1**	
MSC	**180**	**P1**	**(8 years with traditional methods)**
UCLA	**302**	**C2**	
Gramicidin A	317	$P2_12_12_1$	0.3%
Crambin	400	$P2_1$	4%
OCI / U. of T.	**408**	**P1**	**5%**
Rubredoxin	500	$P2_1$	2.7%

Cost-Effectiveness

- Tangent Formula in *SnB*
  - Smaller structures
  - Carefully chosen parameters
- Space Group
  - P1
  - P-1
- Simulated Annealing
- Genetic Algorithms

Running Times

(Average Seconds/Cycle on Iled)

Machine	Total	StrFac	Refine	FFT	Pk Pk
SGI Pwr Ind 2	1.247	0.210	0.426	0.485	0.068
DEC/Alpha	1.822	0.437	0.682	0.520	0.075
SGI Indigo	2.975	0.881	0.760	1.037	0.163
Sparc 10	3.140	0.821	0.919	1.111	0.162
Pentium 75	3.535	1.181	0.995	1.205	0.154
Sparc 5	3.759	0.765	1.087	1.661	0.210
Pentium 90	3.960	1.192	1.172	1.362	0.192
i486dx2-66	11.396	2.175	2.423	5.467	0.711

Additional Applications of *SnB*

- Fragment Recycling (D.A. Langs)
  - Large radius of convergence
  - Superior to traditional tangent formula (RANTAN)
- Electron Diffraction Data (Dorset & McCourt)
  - High success rates
  - Small % of data out of principle plane

Related Presentations

H.A. Hauptman	Last Night	1e.2.A
C.M. Weeks	Monday/Tuesday	M137
G. Prive	Wednesday/Thursday	W008
D. Anderson	Thursday Afternoon	4a.7.A

SnB Addresses

- http://www.hwi.buffalo.edu/SnB
- snb-requests@hwi.buffalo.edu
- snb-comments@hwi.buffalo.edu

Summary

- Alternative structure determination method
- Targeted at 100-800 atom structures
- Publicly available
- Recommend: LEVY / EVAL (Bob Blessing)
- Current Research
  - Parameter tuning / Code Optimization (2X)
  - Additional FOMs
  - Lower resolution data
  - SIR/SAS data