Predefined Molecular Dynamics of Bonded Water Model

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Water structure is:

Immediate-
Vibrational-
Diffused-

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D-structure is: we do not see at every molecule, but to the mosy probable position

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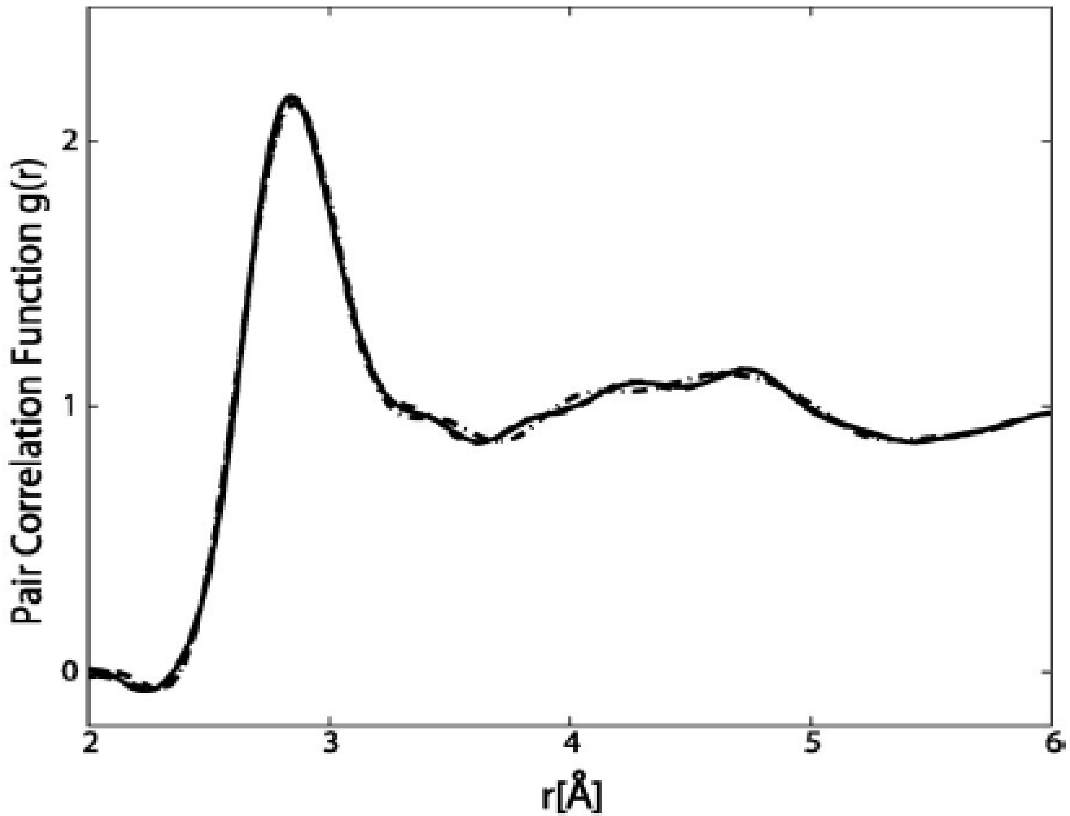
Experiment for D-structure



X-ray structure of liquid water. L. Fu, A. Bienestock, S. Brennan, J.Chem.Phys. 2009, 131

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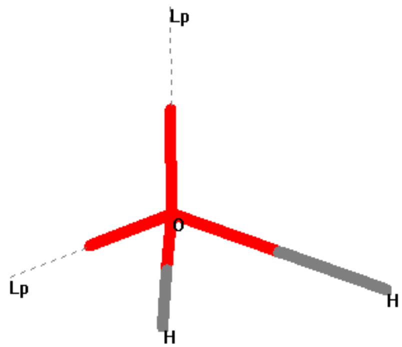
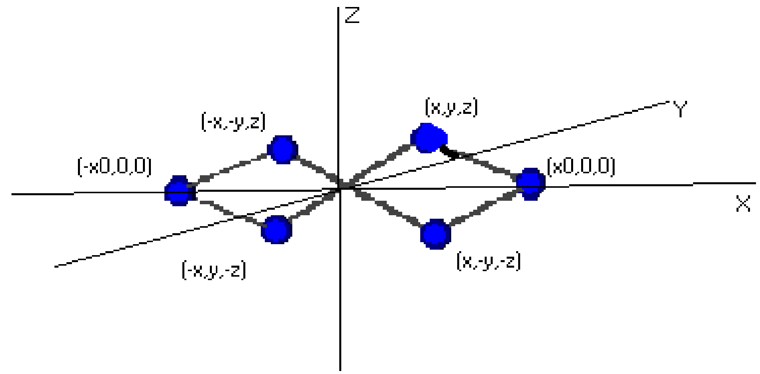
N.A. Bulienkov discontinual model of bonded water: twist-bath





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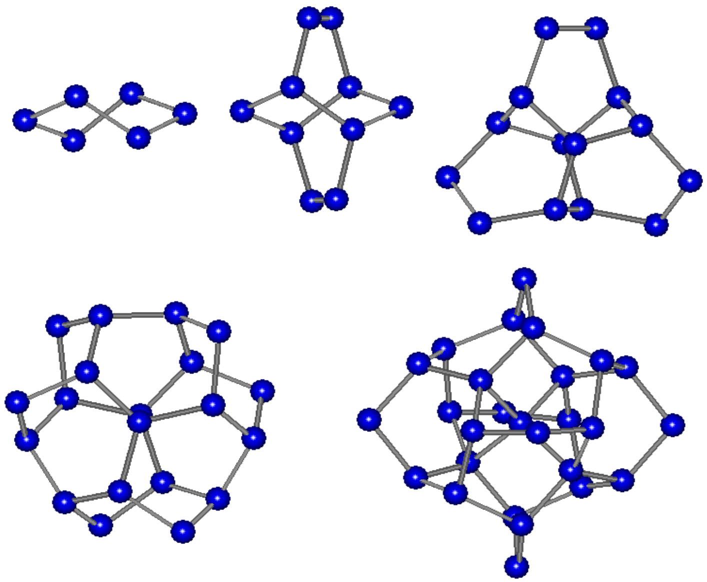
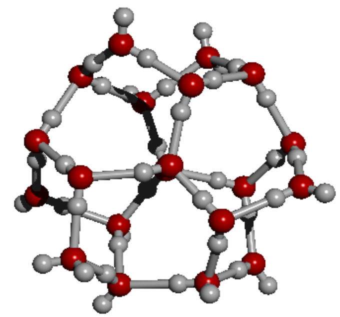
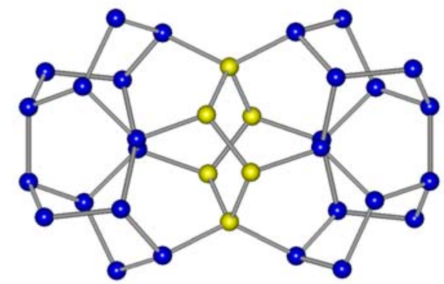
N.A. Bulienkov discontinual model of bonded water: symmetry and construction







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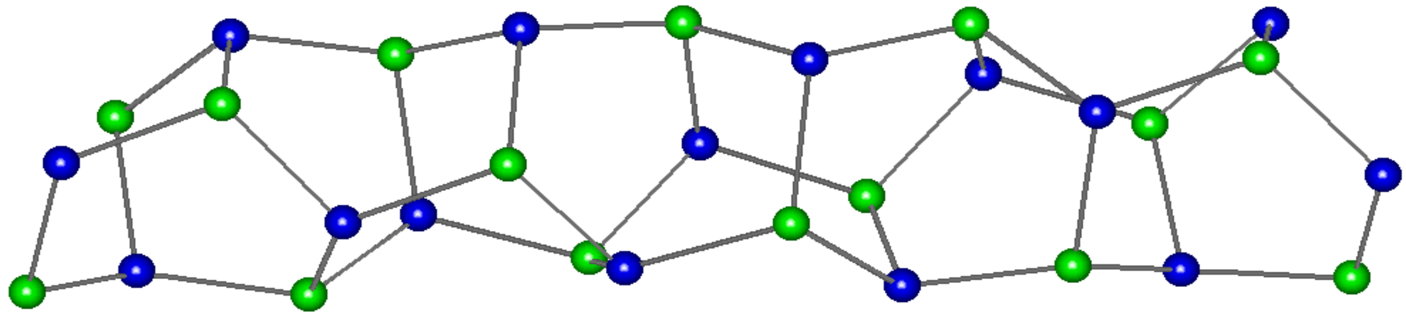
N.A. Bulienkov discontinual model of bonded water:
30/11 helix



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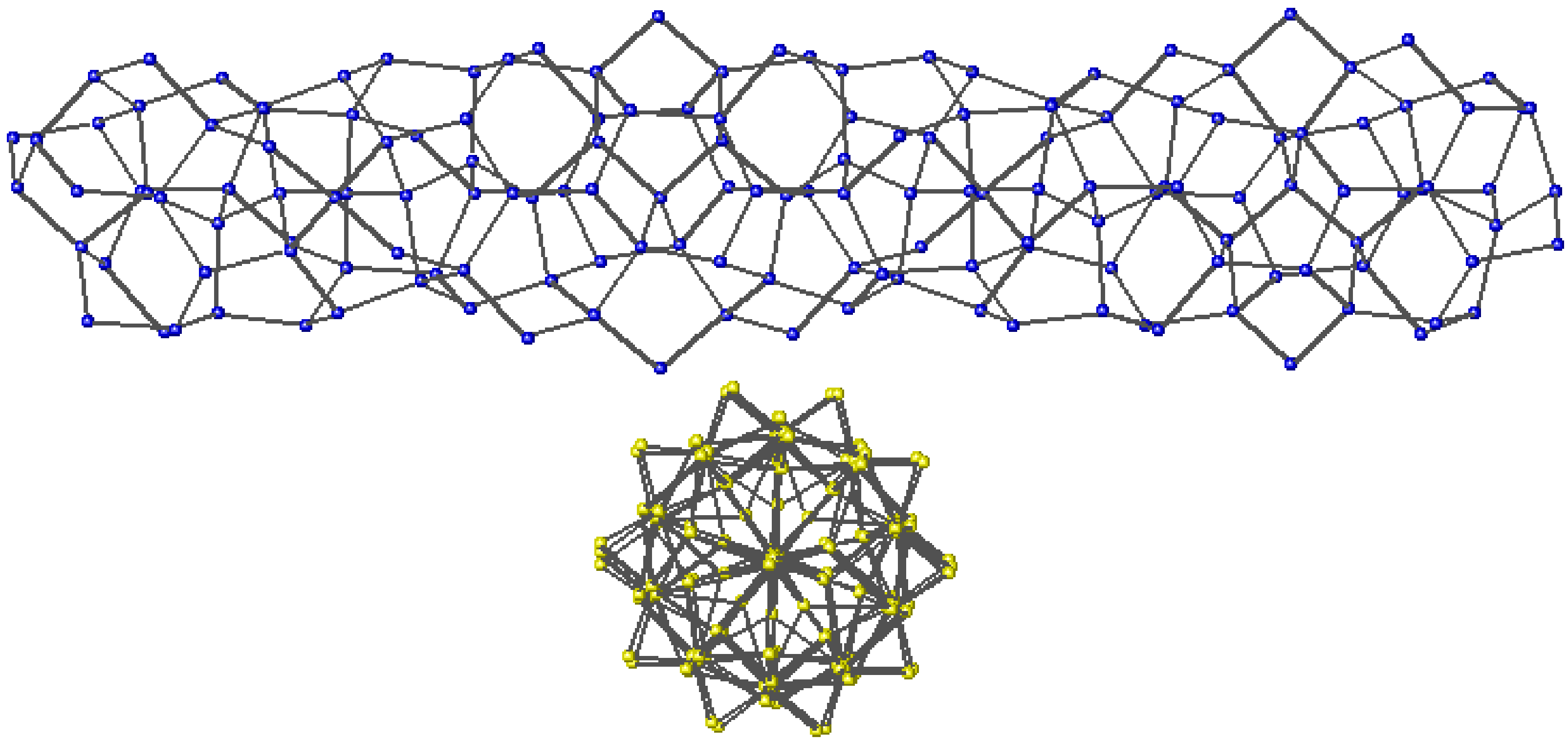
N.A. Bulienkov discontinual model of bonded water:
Non-crystallographic but helical symmetry



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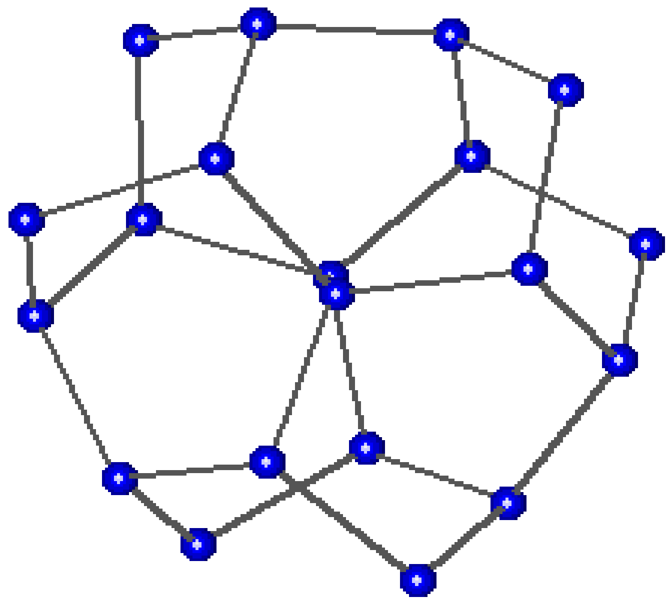
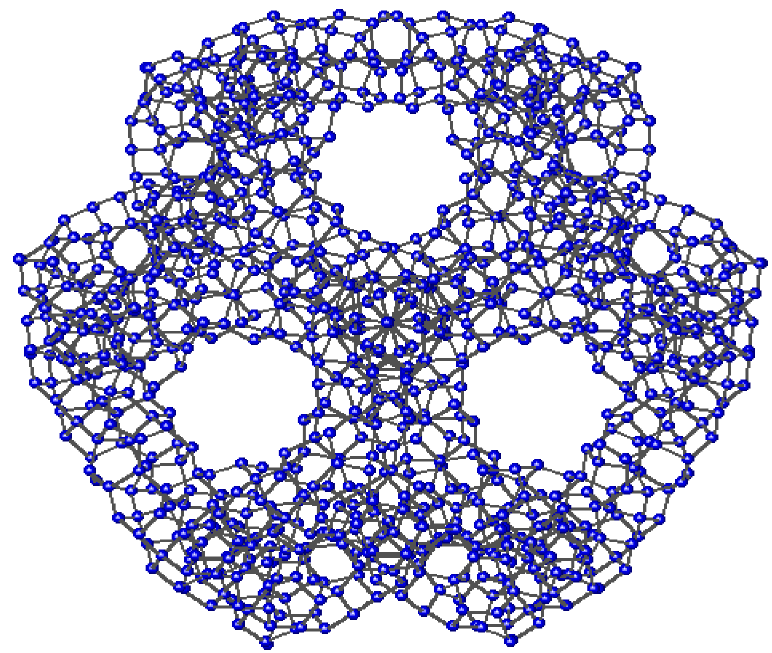
N.A. Bulienkov discontinual model of bonded water: fractals





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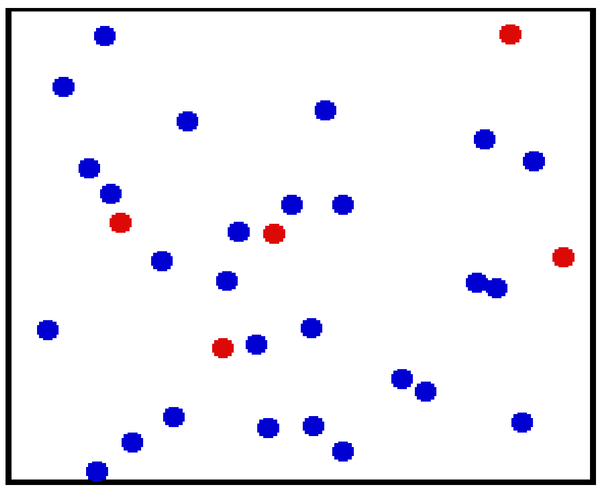
D-structure dynamics?



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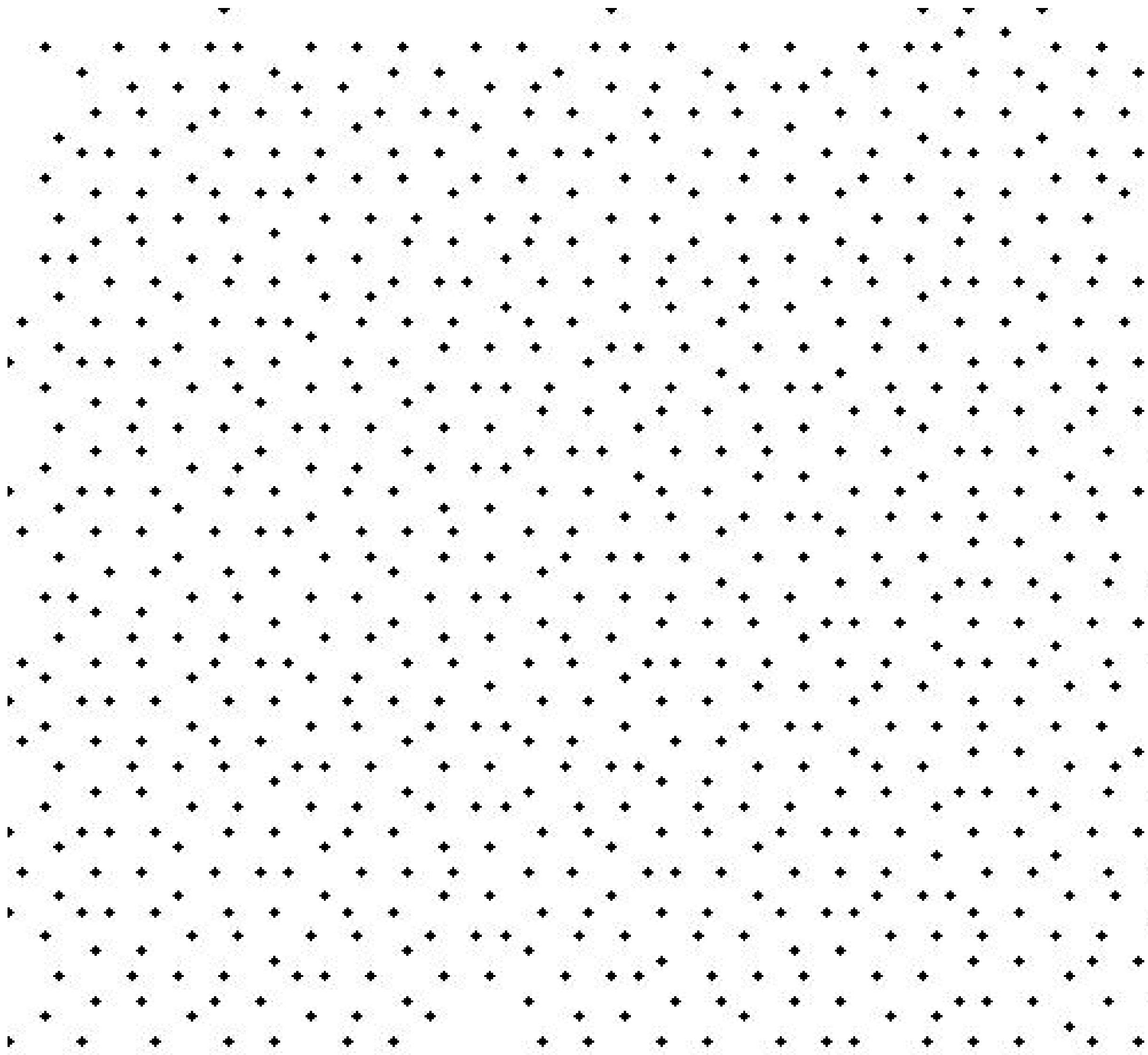

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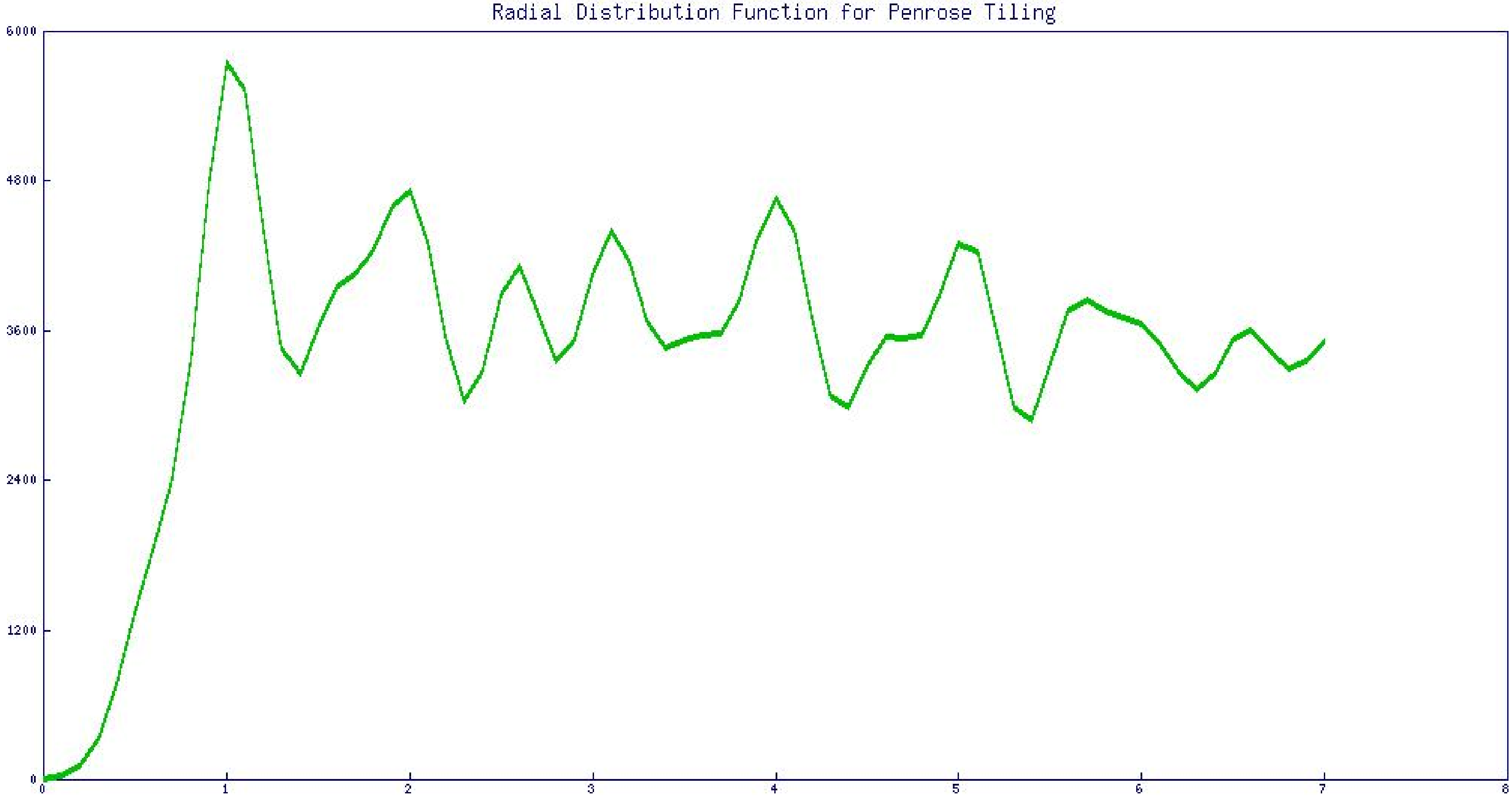

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"The shortest path between two truths on the real line passes through the complex plane."

Jacques Hadamard

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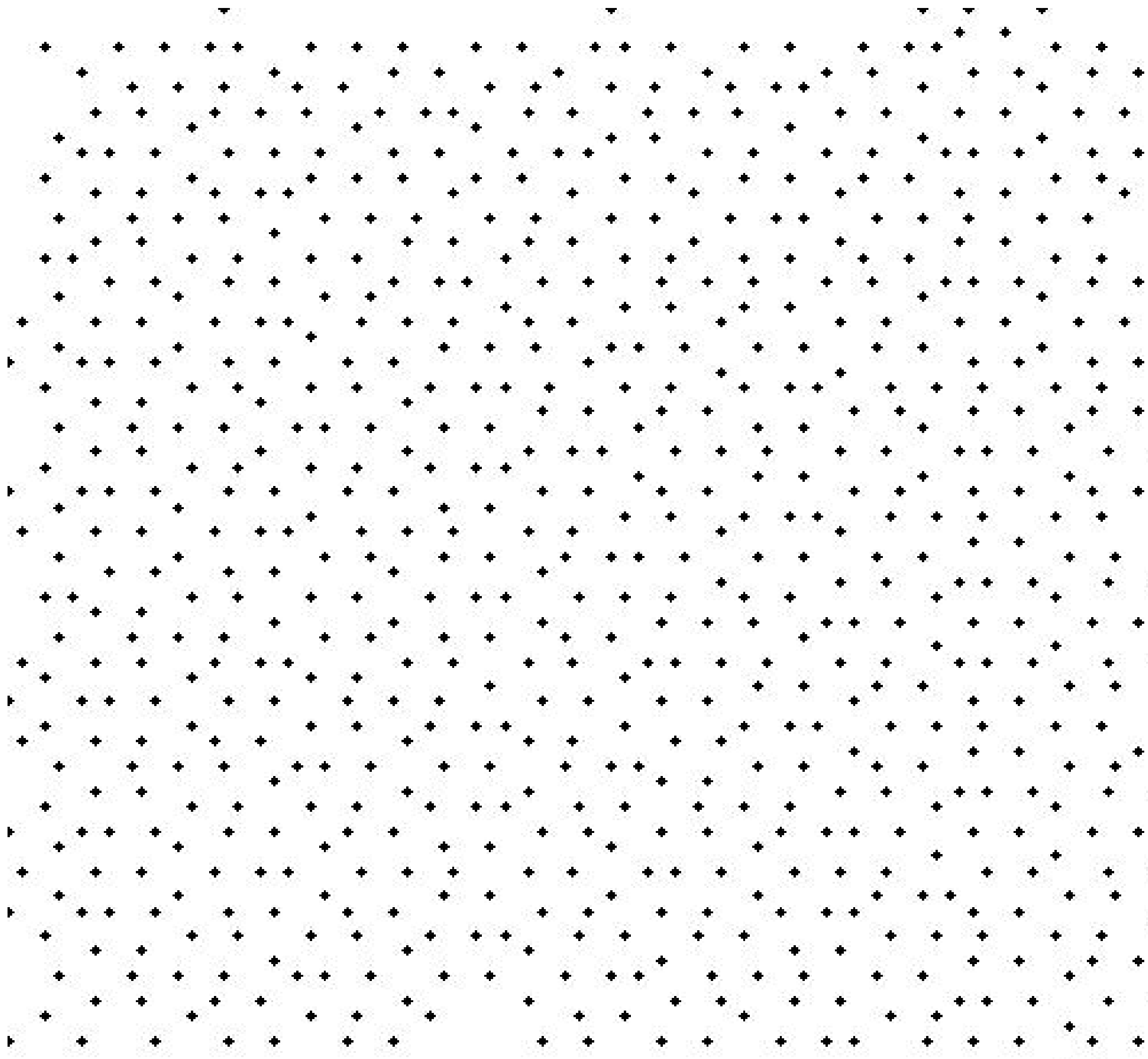

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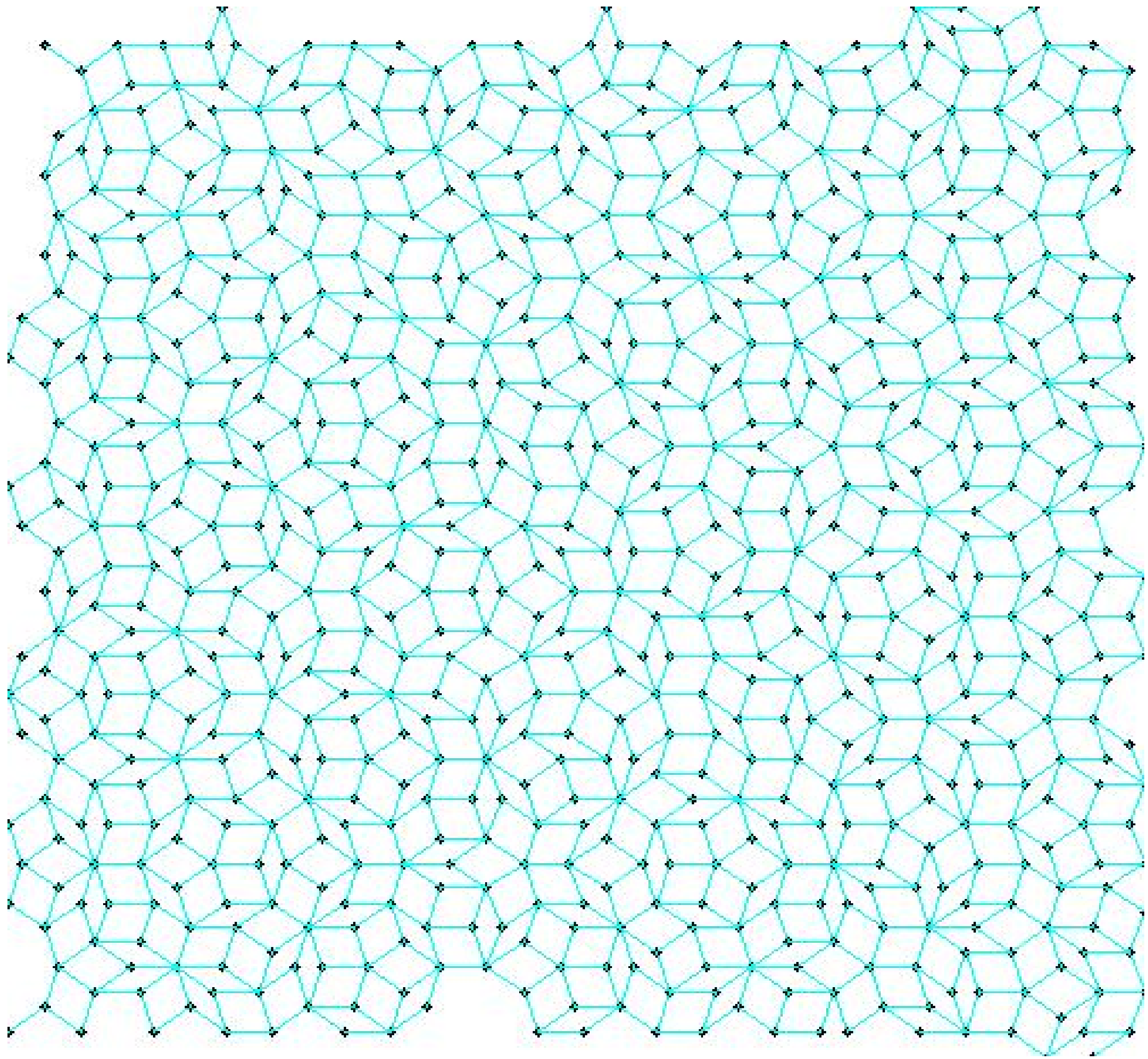

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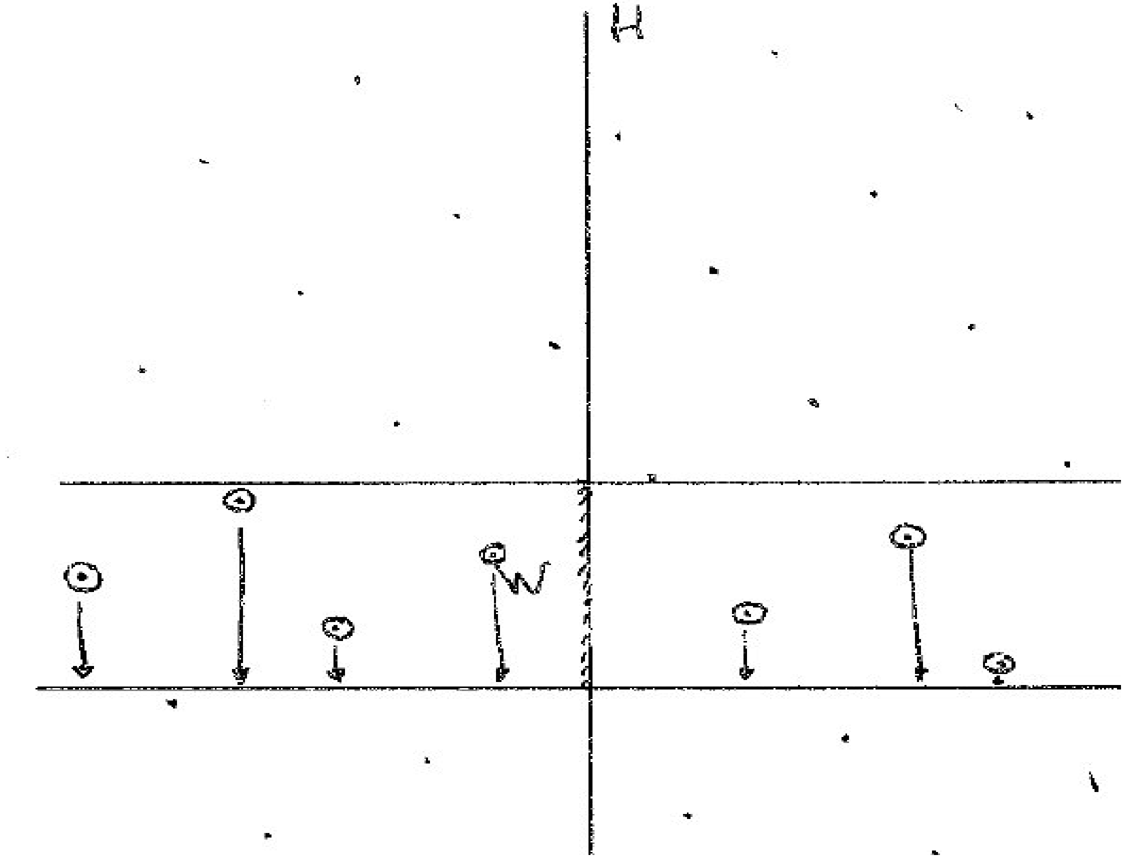

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Predefined dymanics:

1. For D-structure only
2. Projection method from high-dimensional crystal to low-dimensional window using projection
3. Particle jumps provide D-structure geometry evolution.
4. Particle jump occurs when one partice leaves the projection window and another comes in.

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Predefined dymanics:

Preparation step:

1. Select a HD-vector V_move perpendicular to LD-window
   (for example (0,0,1,1,1) perpenducular to (x-y plane)
2. Define N(N-2)/2 angles to rotate HD-lattice

What is D-structure for any $t=\tau$?

3. Rotate HD-lattice, $V(\tau)$ = V_move * τ
4. Leave only particles in window.

In Predefined Dynamics
we do not have to calculate previous step
like in Molecular Dynamics.

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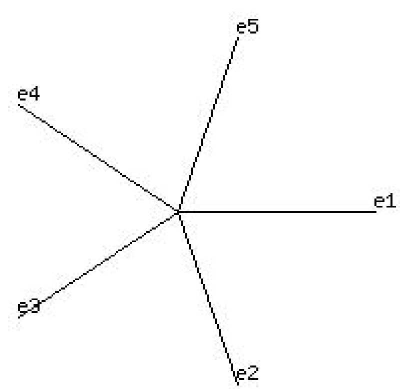
The real water D-structure seems to be tetrahedral and 3D.

But this is too hard (for us) (just for now)
to project 12D crystal down to 3D window

That's why we want to develop the method in 2D.
5D cubic lattice projected to 2D, all basis vectors in projections [e1*,...e5*] are equal. Scalar products are equal too.

|e1*| = |e2*| = |e3*| = |e4*| = |e5*|

(e1* e2*)=(e1* e2*)=(e1* e2*)=(e1* e2*)=(e1* e2*)=cos(2*pi/5)



What about $\langle R \rangle=0$ and $\langle R^2 \rangle \sim t$.

?

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Simple integer 1D Wiener process:

if

$X(0) = 0$

and

$X(t+1) = X(t) \pm 1$ (random jump)

then

$\langle X \rangle = 0$

and

$\langle X^2 \rangle \sim t$

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Irrational projection angle means close-to-random behaviour.

Because of
Irrational
($tg(\alpha) <> N1/N2$)
angles while projection
any particle jumps
randomly
in 5 directions

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Some conclusions are:

Brown motion can be simulated with the Projection method

Penrose tiling can move and changes

Predefined dynamics does not need to calculate prev step

This is up to 2D just for now.

And these are mathimatical tips and tricks.

But they may be useful when studying and modeling real systems cause of their predefined nature

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THANK FOR YOUR ATTENTION!