Supercomputing Applications in Life Sciences

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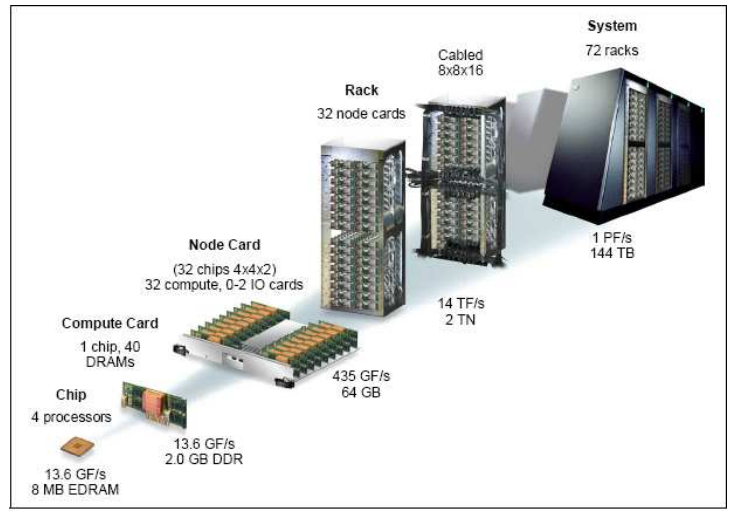
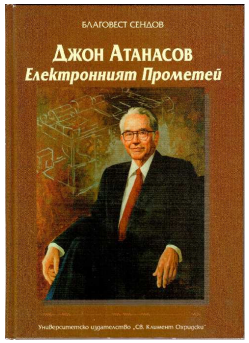
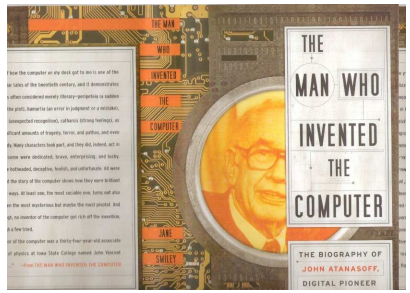
Introduction

- **1961 - The first computer center in Bulgaria is established**
- **2007 - Blue Gene/P is installed at the Bulgarian Supercomputing Centre**







- Atanasoff has been familiar with the numerical method of Ritz leading for his problem to a system of 29 linear algebraic equations.
- Such computations have required many weeks efforts using the Monroe manual rotary Calculator.
- Atanasoff has tried to run several Monroe machines in parallel rotated by a common handle.
- Finally, with a grant of $650 Atanasoff and Berry have created the prototype of the ABC computer in 1939.

B. Sendov, John Atanasoff, The Electronic Prometheus, St. Kliment Ohridski University Press, 2003

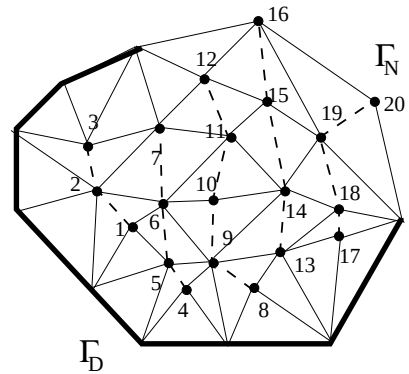
Finite elements method (FEM)

Consider the weak formulation of a given elliptic b.v.p. in the form

$$a(u, v) = \mathcal{F}(v), \qquad \forall v \in \mathcal{V},$$

and the related FEM problem

$$a_h(u_h, v_h) = \mathcal{F}_h(v_h), \qquad \forall v_h \in \mathcal{V}_h.$$



We are interested in the efficient solution of the resulting large-scale FEM linear systems

$$A\mathbf{u} = \mathbf{f}.$$

PCG scalability

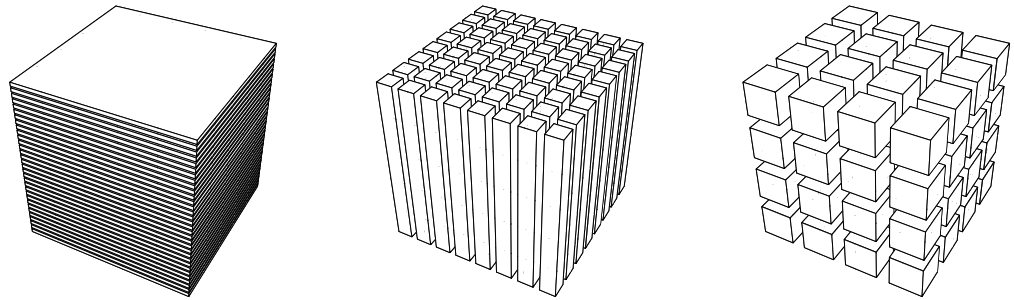
- For large-scale problems, the iterative methods have advantages due to their better/optimal computational complexity and storage requirements.
- The Conjugate Gradient (CG) method is the best iterative solution framework for large scale FEM systems.
- The development of robust Preconditioned Conjugate Gradient (PCG) methods and their parallel implementation is a hot topic in SuperCA.

$h^{-2} \approx N$	DIRECT	CG	PCG-MILU	PCG-AMLI-V	PCG-AMLI-W
1 024	0.02	0.05 (84)	0.04 (21)	< 0.01 (16)	< 0.01 (16)
4 096	0.17	0.12 (163)	0.09 (30)	0.02 (18)	0.02 (17)
16 384	2.21	0.91 (320)	0.52 (46)	0.09 (22)	0.09 (17)
65 536	30.08	9.2 (630)	3.8 (68)	0.49 (25)	0.45 (17)
262 144	*	81.6 (1 256)	27.8 (102)	2.7 (28)	2.3 (17)
1 048 576	*	805 (2 439)	214 (152)	13.3 (31)	10.5 (17)
complexity	$O(N^2)$	$O(N^{3/2})$	$O(N^{5/4})$	$O(N \log N)$	$O(N)$

Solution time in seconds (and n_{it}) for Poisson equation on a unit square

BoomerAMG parallel scalability

Figure: 1D, 2D and 3D partitioning: voxel triangulation of a cubic domain



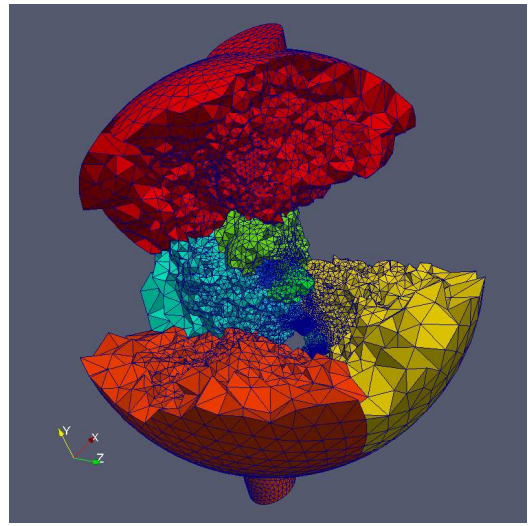
Parallel numerical tests based on BoomerAMG solver for a parabolic problem in a cubic space domain, voxel FEM mesh, and 96 implicit backward Euler time steps, are given bellow.

Parallel scalability

Mesh	$N_p = P_x \times P_y \times P_z$	N	N_{it}	T(p) [s]	E(p)
127 x 127 x 127	*8 = 8 x 1 x 1*	*2 097 152*	*161*	*1 255.00*	
255 x 255 x 255	*64 = 64 x 1 x 1*	*16 777 216*	*128*	*5 951.08*	*21 %*
511 x 511 x 511	*512 = 512 x 1 x 1*	*134 217 728*	*-*	*> 24* h	*< 2 %*
127 x 127 x 127	*8 = 4 x 2 x 1*	*2 097 152*	*167*	*1 137.83*	
255 x 255 x 255	*64 = 8 x 8 x 1*	*16 777 216*	*129*	*1 203.29*	*95 %*
511 x 511 x 511	*512 = 32 x 16 x 1*	*134 217 728*	*114*	*1 581.13*	*72 %*
127 x 127 x 127	*8 = 4 x 2 x 1*	*2 097 152*	*167*	*1 137.91*	
255 x 255 x 255	*64 = 4 x 4 x 4*	*16 777 216*	*128*	*1 062.30*	*107 %*
511 x 511 x 511	*512 = 8 x 8 x 8*	*134 217 728*	*114*	*1 155.08*	*99 %*

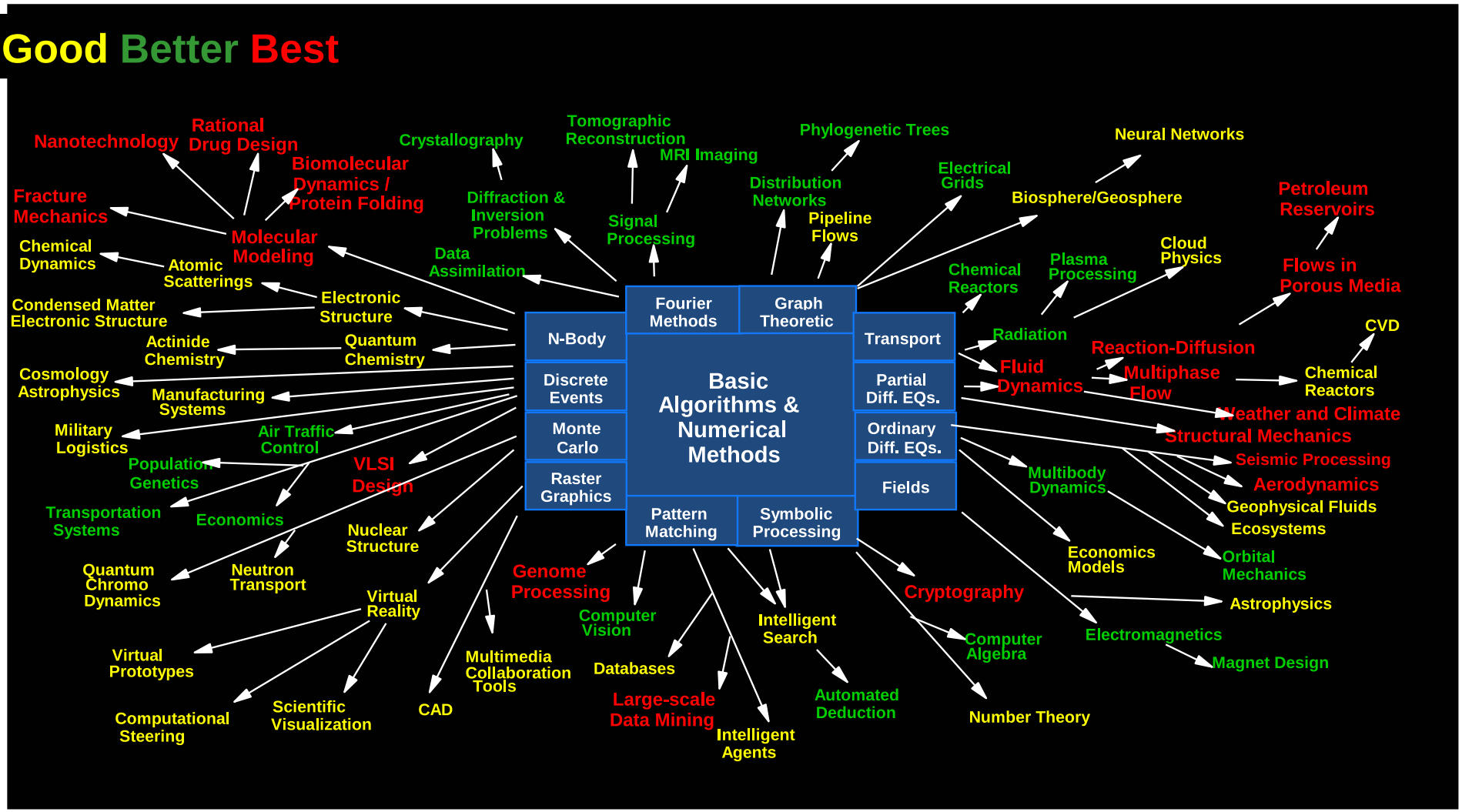
Parallel FEM tools

- mesh generation (NetGEN)
- domain partitioning (ParMETIS, SCOTCH)
- parallel solver (BoomerAMG)
- parallel Multiphysics ELMER



Domain/graph partitioning of unstructured mesh for 16 processors

Supercomputing applications

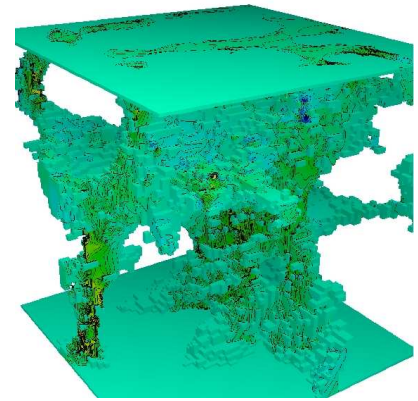


Argonne National Labs GBB

Bone microstructure

- μFEM analysis with NC Rannacher-Turek FEs is applied in a voxel setting.
- solid skeleton at micro level $\Rightarrow$ anisotropic tensor at macro level.
- MIC(0) and BoomerAMG in combination with Displacement Decomposition.

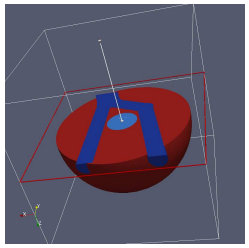
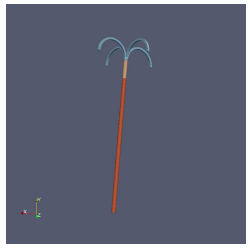
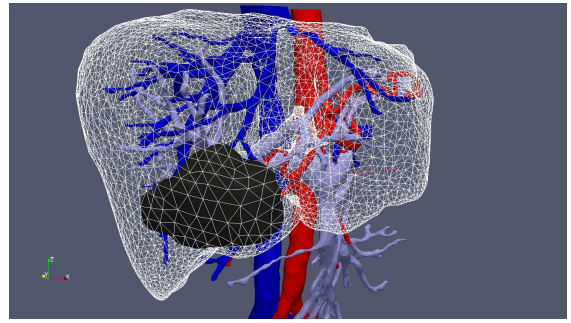
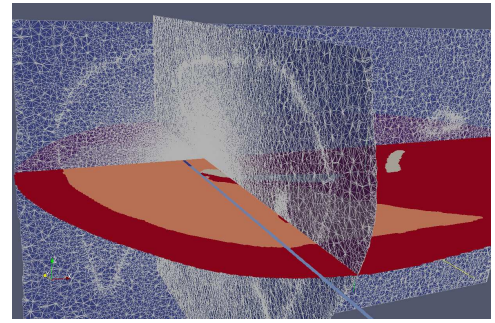
		$\zeta = 0.1$			
		MIC(0)		AMG	
n	p	$T[s]$	It	$T[s]$	It
64	1	1 184	270	1 071	28
128	8	1 831	395	1 147	25
256	64	4 870	888	1 318	25



		$\zeta = 0.01$			
		MIC(0)		AMG	
n	p	$T[s]$	It	$T[s]$	It
64	1	2 634	601	2 384	63
128	8	4 905	1 060	2 860	63
256	64	10 177	1 863	2 715	52

		$\zeta = 0.001$			
		MIC(0)		AMG	
n	p	$T[s]$	It	$T[s]$	It
64	1	4 477	1 022	4 412	117
128	8	9 626	2 081	5 928	131
256	64	16 182	2 965	6 939	102

RF tumor ablation

- **The RF ablation destroys the unwanted tissue by heating, arising when the energy dissipated by the electric current flowing through the RF probe is converted to heat.**

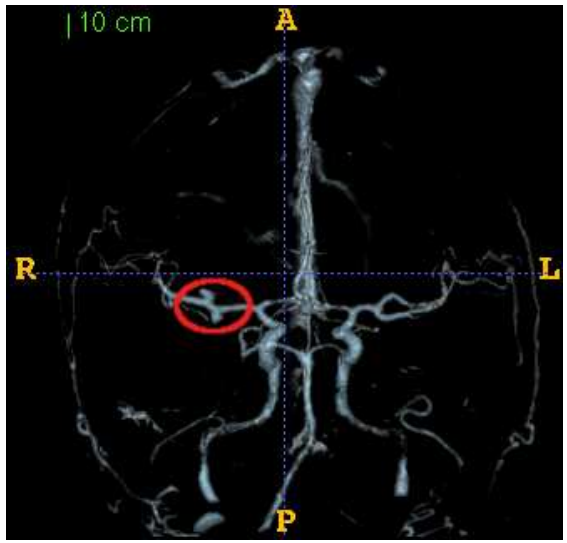
	Degrees of freedom (DOF)		
n_p	2 097 152	16 777 216	134 217 728
32	1 788		
64	884		
128	457		
256	250	1 880	
512	165	1 107	
1 024	155	667	
2 048	387	708	3 340

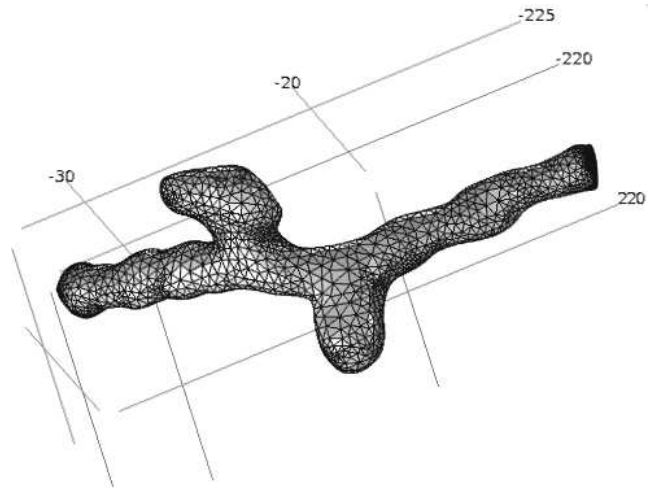
Parallel times T[s] for simulation of 8' of HTA with time step of 1"

Cerebral aneurysms

Towards realistic simulation of cerebral aneurysms:

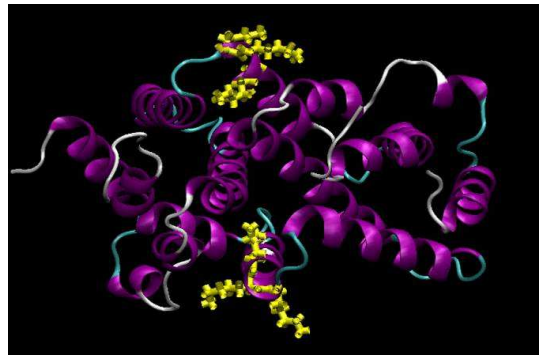
- **Patient specific computed tomography data**
- **Parallel software tools for CFD simulation**

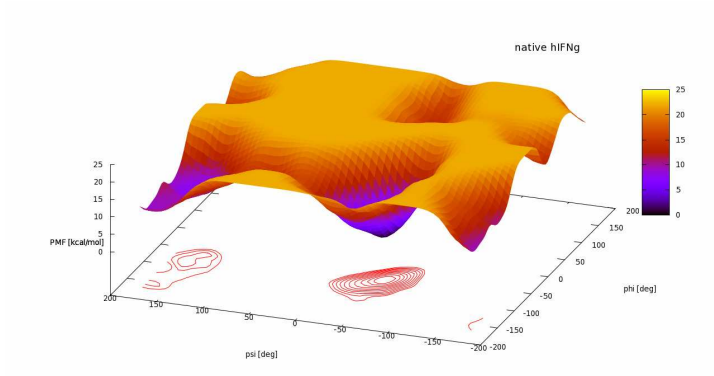




Human interferon gamma

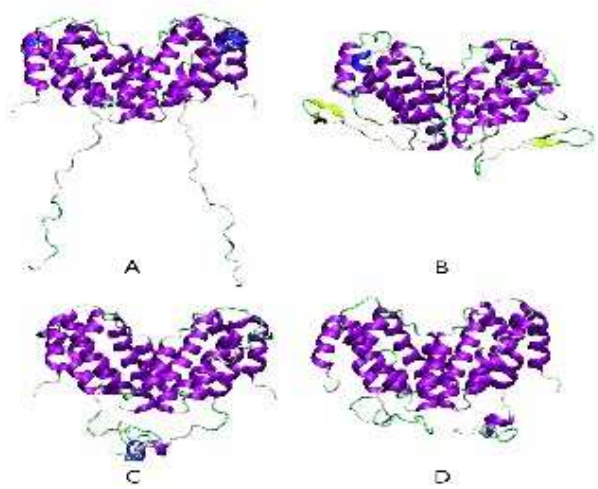
- The structural stability of 100 hIFNg mutants with 3 random mutations in the upstream NLS (aa 86-89) are studied using metadynamics based on collective variables the backbone dihedral angles of the 86-th amino acid.
- The free energy profile of the native and mutated forms of the protein are reconducted by comparing the profiles to the native form.





Conformation of C-terminus

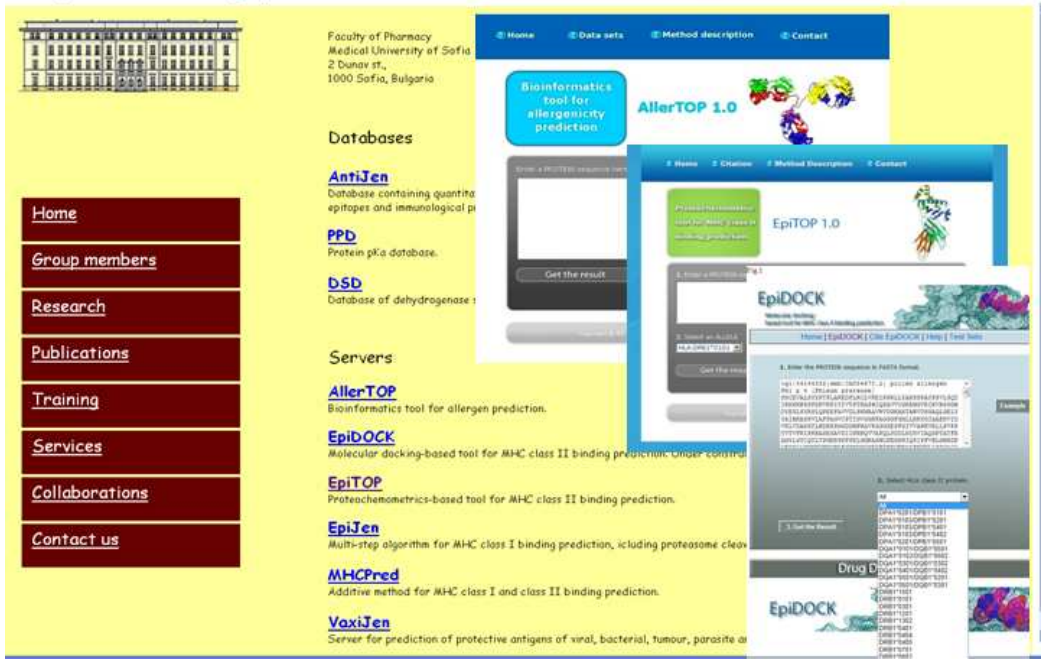
- The length of the tail modifies the affinity to the receptor.
- Two 200 ns MD folding simulations are performed using GROMOS 53a6 + GROMACS 4.5.4 and CHARMM 22 + NAMD 2.9 to cluster the trajectories.
- It was found that in both cases the C-Termini get closer to the globule and the whole protein adopts more compact conformation.



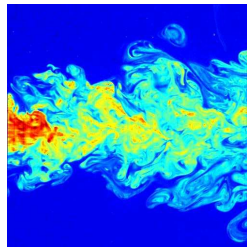
In silico drug design

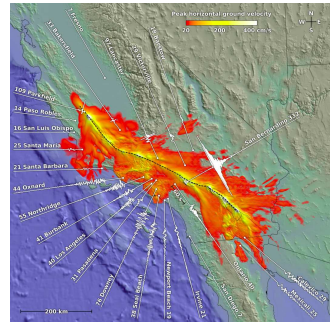
- **Structure-based methods for drug design are used to develop models for allergenicity and immunogenicity predictions of novel proteins.**
- **Molecular dynamics simulations and molecular docking studies are applied on BlueGene-P to derive the models.**
- **Once the models are derived, they are freely accessible via the web site:**

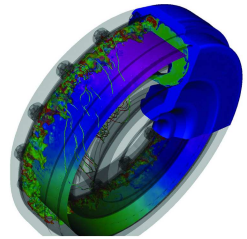
http://www.ddg-pharmfac.net

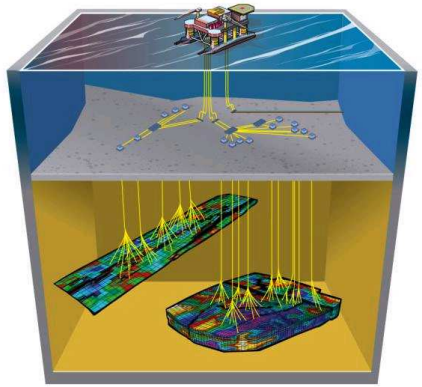


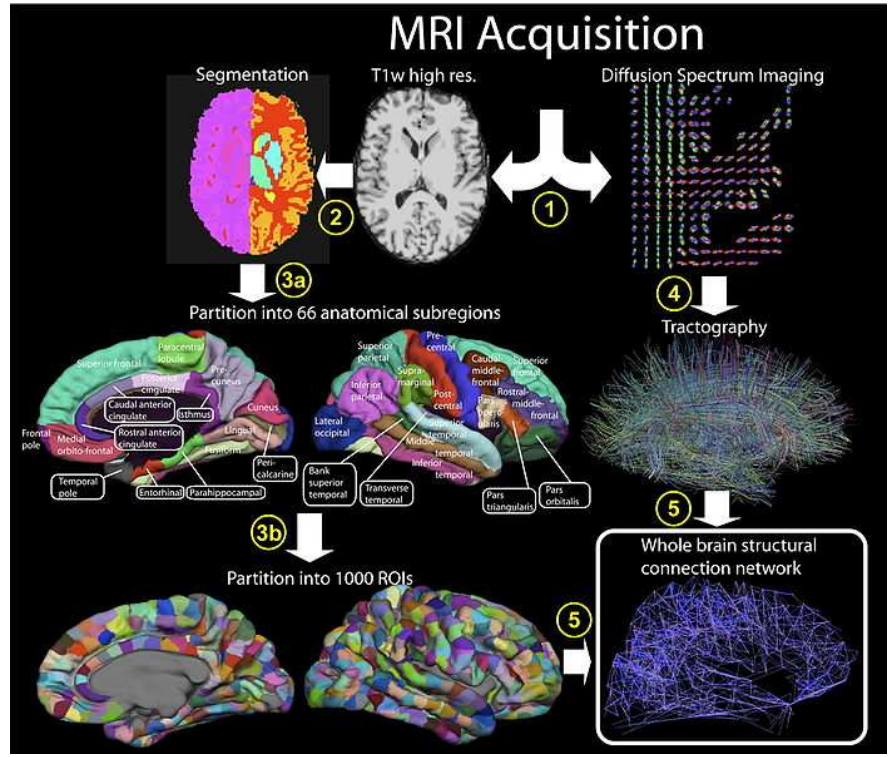
Advanced SC applications











Supercomputing in Blue

- **Blue Gene/P: 4 x 3D Torus:**
- **Blue Gene/Q: 32 x 5D Torus**
- **Blue Water: diam = 4**

Theory and practice

- ”There is nothing so practical as the good theory.”

  Kurt Lewin

- ”In theory, theory and practice are the same. In practice, they are not.”

  Albert Einstein

THANK YOU !

Acknowledgments:

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