

SIMULATIONS FOR RNA WITH DIVERSE SCALES AND ASPECTS

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MULTISCALE MODELING

Multiscale modeling uses mathematics and computation to quantitatively represent and simulate a system at more than one scale while functionally linking the mathematical models across these scales.

The NIH, DOE, FDA and NSF recognize that to efficiently and effectively address the challenges of understanding multiscale biological and behavioral systems, research will need predictive, computational models that encompass multiple biological and behavioral scales.

There is a funding opportunity announcement at grants.nih.gov/grants/guide/pa-files/PAR-11.203.html
DC : limit \$500,000 per year ; expected \$200,000 - \$400,000 per year, plus indirect

Remaining due dates : 05/31/13, 09/27/13, 01/31/14.



AMYOTROPHIC LATERAL SCLEROSIS RESEARCH PROGRAM THERAPEUTIC IDEA AWARD

No preliminary data needed.

Investigators at all academic levels are eligible.

Idea to be proposed :

- Use “spared” neuron type to make pluripotent stem cell. [KHM12]
- Inject into ventral horn [inj, GBJ⁺12]
- Encourage existing neuron to guide developing neuron to site [OFH⁺13][WMGG⁺12][RFW⁺12][FPIS12]
- Induce new neuromuscular junction [LZM⁺12]

There is a funding opportunity announcement at
cdmrp.army.mil/funding/alsrp.shtml

DC : maximum \$400,000 total, plus indirect, negotiated rate

Remaining due dates : June 5, 2013, pre-application. (Application by invitation, Sept. 18, 2013)



Differential gene expression in “spared” and vulnerable motor neurons

Want to analyze differential expression data

Classify the collection of reads, as arising from a mixture of processes of gene expression

Topic models (Blei) might be useful

Develop control network (faculty candidate)

Calculate intervention

Translate into clinical therapy

RNA HEXANUCLEOTIDE REPEATS IN INTRON

In C9ORF72

- a hexanucleotide repeat [MWA⁺¹³] “leading to abnormal RNA splicing”
- ligands bind to the repeats

RNA METABOLISM SOFTWARE

Simulations for
RNA
with Diverse
Scales and Aspects

Thérèse Smith

Name	(Scale or Aspect) and Purpose
NAMD	atomic, simulation
AMBER	atomic, force field to accompany NAMD
RUM	base, RNA-seq alignment
RNALSOpt	secondary structure, stable, local, optimal (riboswitches)
IQSeq	base/molecular, isoform quantification
gfold	molecular, topology
HADDOCK	molecular, docking
Stanford Topic Modeling Toolbox	classifying reads (especially motifs with matching sequences) as to gene expression process
bioconductor (PUMA)	gene expression profiles want to modify with topic model approach
MAMMOTH	model comparison



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