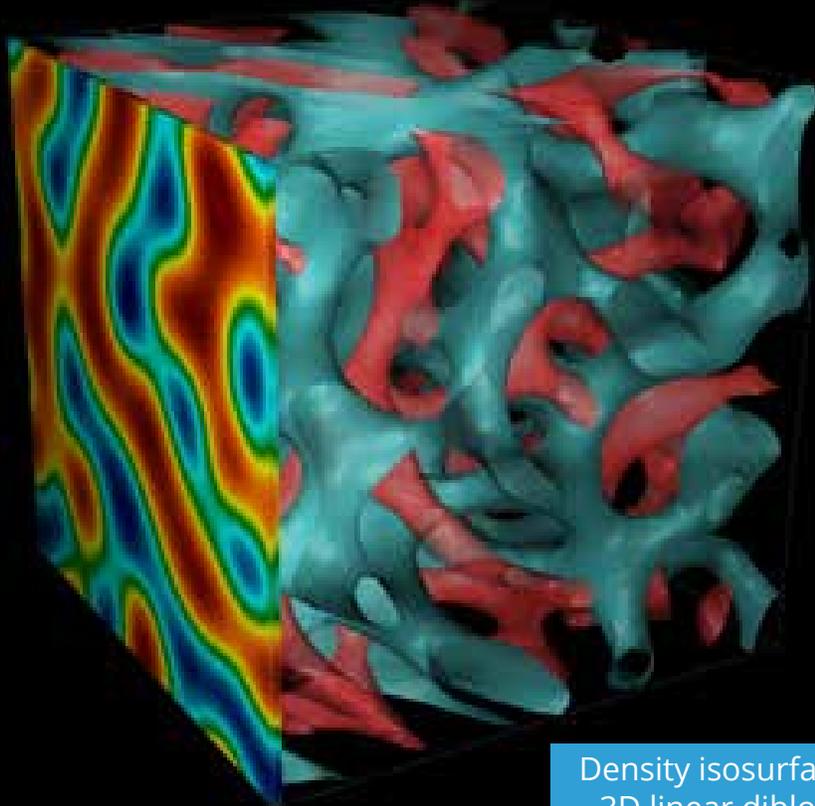


# PSim

Faster simulations of complex block copolymer mixtures.



PSim enables researchers to model complex block copolymer mixtures at the mesoscopic level critical to many nanoscience applications. PSim provides a flexible simulation tool for studying the mesoscale structure of complex polymeric materials by combining self-consistent field theory (SCFT) methods with high-performance computing.



Density isosurfaces for phase-segregating 3D linear diblock from embedded VisIt.

## Mesoscale Simulations

PSim is a powerful method for studying the complex morphologies of multi-component block copolymers and nanocomposite mixtures. The simulation tool supports a systematic coarse-graining of length scales at the molecular level to efficiently study mesoscopic features not easily accessible to explicit, particle-based methods.

## Scalable Simulations for Your Hardest Problems

*Since PSim supports massively parallel computing and scales to hundreds of processor cores, new problems that were previously unsolvable are now within reach. PSim works on Linux, Windows, and Mac OS X platforms. Our competitive pricing means that the more computing cores you need, the less you pay per core, whether you use batch computing on clusters, or large single computing jobs.*

[www.txcorp.com](http://www.txcorp.com)

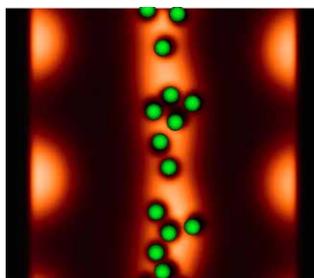
[sales@txcorp.com](mailto:sales@txcorp.com)  
5621 Arapahoe Ave | Boulder | CO 80303  
Telephone: +1-303-448-0727

## PSimBase Features:

- Multi-block linear copolymers
- Arbitrary branched copolymers
- Distributed memory parallelism
- Neutral, flexible chain model
- Mixtures of copolymers, homopolymers and solvent species
- Histories
- Spectral filtering
- Zone annealing

## PSimPlus Includes All PSimBase Features PLUS:

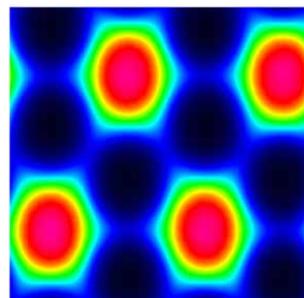
- Specify arbitrary geometry for surfaces/ confinement
- Hybrid-SCFT for explicit nanoparticle composites
- Specify Flory-type interactions for nanoparticles/ surfaces
- Patterned surface interactions



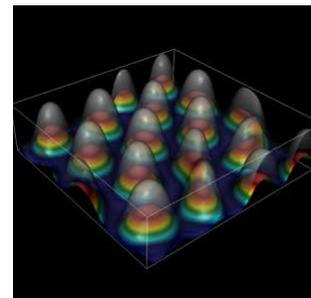
*2D block copolymer and nanoparticle mixture. The nanocomposite mixture is confined between parallel, flat surfaces. This simulation utilizes the hybrid-SCFT method in PolySwift++ for explicitly including the effects of embedded nanoparticles.*

## Consulting Services

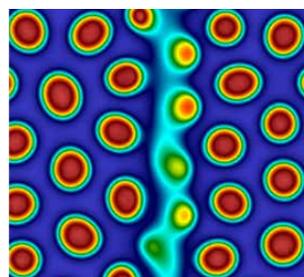
Tech-X offers consulting and training services for all of its simulation software. In addition to the free support that comes with every purchase of a PSim product, we have our experts ready to help you use PSim to its fullest possible extent to solve your most challenging problems.



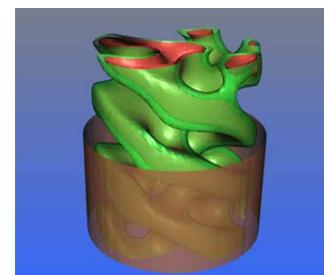
*Monomer density plot for an ABC star-copolymer.*



*Projected density values for phase-segregated linear ABA triblock. The total A monomer density is tracked separately from the contribution from one of the A endblocks.*



*Intermediate morphology for a linear AB diblock. A slab 'zone' is moving through the simulation grid that simulates local heating. This zone-annealing technique can also be used to speed relaxation to the equilibrium structure much like in real experimental situations.*



*3D density isosurfaces for a linear diblock in cylindrical confinement. A cutaway view of the cylindrical confinement is shown as a brown isosurface.*

PSim and Tech-X are registered trademarks of Tech-X Corporation. All other trademarks are the property of their respective owners.

## About Tech-X Corporation

Tech-X Corporation is committed to technical excellence and innovation. Our scientists and software engineers work together to deliver quantifiable results. We combine academic research with a commercial software company sensibility to deliver high-quality, cutting-edge software that takes advantage of the latest hardware and software advances.